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INTERNATIONAL CONFERENCE ON PORPHYRINS & PHTHALOCYANINES

28 JUNE - 3 JULY 2026

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BOOK OF ABSTRACTS

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Preface

In this book are gathered together all the abstracts of presentations given at the Fourteenth International Conference on Porphyrins and Phthalocyanines (**ICPP14**) 28 June - 3 July 2026 in Kyoto, Japan as the first physical ICPP meeting since the pandemic.

The PDF version of this Book of Abstracts is also available online on the ICPP website.

645 particpants from **38** different countries have contributed for a total of **597** abstracts.

This book summarizes the most recent activities in porphyrins, phthalocyanines and related macrocycles by members of our society.

The abstracts are divided into three categories as described below:

Award Lectures (**8**)
Oral Presentations (**404**)
Poster Presentations (**185**)

The papers associated with the abstracts are presented in **40** specialized symposia, organized by **106** symposium organizers.

The program book, available to each participant is available online and contains all the information of each presentation as well as the weekly schedule.

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Matthew Padgett - SPP Office, Dijon, France : icpp@spp-jpp.org



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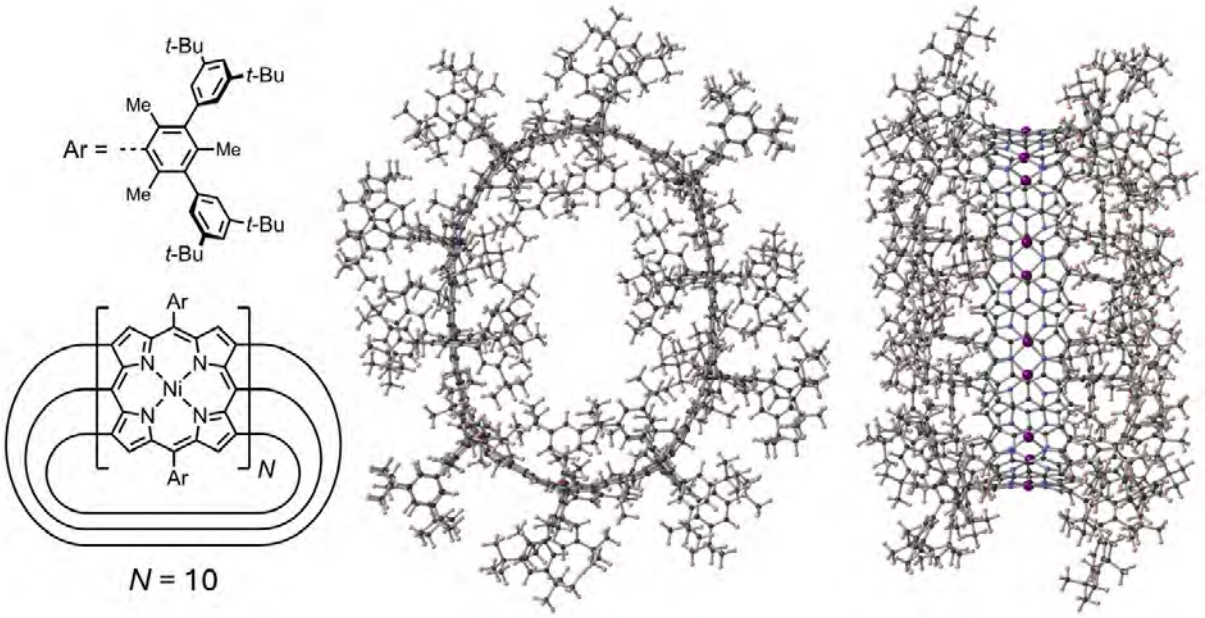
AWARDS

Porphyrin-Based Molecular Wires, Nanorings and Nanobelts

Harry L. Anderson

University of Oxford, United Kingdom

Molecular wires are the simplest single-molecule electronic devices, and they can be viewed as the elementary components of bulk organic semiconductors. Molecular wire rings exhibit fundamentally different behavior from straight molecular wires, leading to the phenomenon of aromaticity [1]. This lecture will present the synthesis and investigation of several linear and cyclic molecular wires based on porphyrins, with emphasis on understanding electronic delocalization in longer chains and larger rings. The rigid structures of porphyrins lead to small reorganization energies, leading to low barriers for charge transport and electronic delocalization [2]. The presentation will include recent work on triple stranded porphyrin nanobelts, such as the 10-porphyrin nanobelt shown in the graphic below (X-ray crystal structure) [3].



REFERENCES

1. M. Jirásek, H. L. Anderson, M. D. Peeks, From macrocycles to quantum rings: Does aromaticity have a size limit? *Acc. Chem. Res.* **2021**, *54*, 3241–3251.
2. J.-R. Deng, M. T. González, H. Zhu, H. L. Anderson and E. Leary, Ballistic conductance through porphyrin nanoribbons. *J. Am. Chem. Soc.* **2024**, *146*, 3651–3659.
3. A. Rodríguez-Rubio, H. Zhu, K. M. Cheung, I. Rončević, L. A. Gödde, J. Hergenhahn, J. L. Field, P. Gupta, W. Stawski, H. Gotfredsen, J. Straw, M. Edmondson, J. O'Shea, A. Saywell, H. L. Anderson, Synthesis of triple stranded porphyrin nanobelts. *Science* **2025**, *390*, 290–293.

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AWARDS

Bio-inspired Supramolecular Electron and Energy Transfer: Design Perceptions for Producing High-Potential, Long-Lived Charge Separated States

Francis D'Souza

[a]*Departments of Chemistry and Materials Science and Engineering, University of North Texas, 1155 Union Circle, #305070, Denton, TX 76203-5017, USA; E-mail: Francis.Dsouza@unt.edu*

The construction of supramolecular systems capable of mimicking biological functions, whether through self-assembly or covalent bonding, is one of the fastest-growing and most fascinating areas of research. In this regard, the construction of donor-acceptor conjugates capable of undergoing electron or energy transfer upon photoillumination holds great promise for light energy harvesting, nanotechnology, sensing, and the design of optoelectronic devices. Mimicking the primary events in the antenna and reaction centers of photosynthesis is an important area of research, as it directly involves converting solar energy into electricity or making fuels for a sustainable society. Several elegant tetrapyrrole-derived supramolecular systems have been designed and studied for these applications.

This award talk summarizes the progress made in our laboratories over the years on tetrapyrrole-derived donor-acceptor conjugates. In our construction, porphyrin, phthalocyanine, and BODIPY have been primarily used as electron donors or excitation-transfer agents. In contrast, all carbon-derived materials, including fullerene, carbon nanotubes, graphene, and other two-dimensional electron-deficient molecules, such as tetracyanobutadiene and perylenediimide, have primarily been used as electron acceptors. Apart from covalent linkage, self-assembly protocols involving cation-dipole, dipole-dipole, hydrogen bonding, metal-ligand coordination, and $\pi-\pi$ interactions have been successfully employed in the construction of these conjugates. The effects of distance and orientation, the role of intermolecular forces in governing the stability and geometry of the nanoconjugates, and their significance in controlling kinetics and mechanism of electron- and energy-transfer events, especially in generating high-potential, long-lived charge-separated states, much desired for photocatalytic applications, will be highlighted.

The author is thankful to all his past and present graduate and undergraduate students, post-doctoral fellows, collaborators, and visiting scholars. He is also grateful to the funding agencies, ACS-PRF, NSF, DOE, NIH, and NSF-EPSCoR, for financial support. Institutional support from the University of North Texas, Denton, Texas, and Wichita State University, Wichita, Kansas, and all collaborators' institutions, is duly acknowledged.

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Modification of Hemoproteins for Creating New Biocatalysts and Bionanomaterials

Takashi Hayashi

Graduate School of Engineering, The University of Osaka, Japan

Hemoproteins are widely distributed in nature and function as small molecule binders, electron carriers, catalysts, sensors/regulators and more. These functions primarily arise from the properties of the heme cofactor and its surrounding coordination sphere, which is composed of proteins. Over the past few decades, numerous hemoproteins have been discovered and identified [1]. Futhermore, the introduction of site-directed mutations into hemoproteins has accelerated the elucidation of their functional mechanisms. Furthermore, some hemoproteins can be converted to their apoforms by removing the cofactor from the heme pocket, making it possible to reconstitute hemoproteins by adding artificial metallocofactors into the apoprotein solutions. Several groups have incorporated modified iron porphyrins into hemoproteins, such as myoglobin to elucidate protein functions based on the interaction between the heme cofactor and the heme pocket. In contrast, for over 30 years, our group has amined to modify the hemoprotein functions by replacing native heme with artificial heme derivatives to create new biocatalysts and bionanomaterials. This presentation introduces several representative examples of our reconstituted hemoproteins as shown below [2-3].

1. Enhancement of myoglobin or peroxidase fuctions
   Myoglobin and horseradish peroxidase reconstituted with iron porphycene were confirmed to exhibit enhanced O_2 affinity and peroxidase activity, respectively.

2. Elucidation of the heme-propionate side chains in P450cam
   A single-legged heme cofactor where one of the heme-propionate side chains was replaced with a methyl group clearly indicated the role of the interaction between the heme side chain and the protein in P450cam.

3. Modeling of methionine synthase or methyl-coenzyme M reductase
   Myoglobins reconstituted with cobalt corrin and nickelt corrin derivatives demonstrated the structural and functional models of the enzymes, respectively.

4. Creation of new artificial metalloenzymes
   Using metalloporphyrinoids as artificial cofactors, myoglobin was converted into artificial metalloenzymes such as hydroxylase, cyclopropane synthase, nitrile synthase.

5. Formation of hemoprotein assembly
   Artificial hemoprotein assemblies (named “hemoprotein polymers”) were created using apohemoproteins in which heme derivatives were covalently linked onto the protein surface.

REFERENCES

1. T. Hayashi, in *Handbook of Porphyrin Science*” Eds. K. M. Kadish, K. M. Smith, R. Guilard, World Scientific (Singapore), 2010, Vol. 5, Chapter 23, pp 1–69.
2. K. Oohora, A. Onoda, T. Hayashi, *Acc. Chem. Res*., **2019**, *52*, 945–954.
3. T. Hayashi, *Bull. Chem. Soc. Jpn*., **2023**, *96*, 1331–1338.

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AWARDS

Bio-inspired Fe porphyrins as the best catalysis of the reduction of O_2 contradict the Sabatier-Principle volcano correlation of activity versus MN4-O_2 binding energy

José H. Zagal-Sagal[a], Laura Scarpetta-Pizo[a], Wolfgang Schmickler[b]

[a]*Laboratory of Electrocatalysis and Molecular Electronics, University of Santiago de Chile, Santiago 970000*
[b]*Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm*

This manuscript discusses several strong limitations in applying the Sabatier Principle to interpret the catalytic activity of graphite-surface-confined macrocyclic metal complexes in the O_2 reduction reaction in 0.1 M NaOH. Many volcano correlations in the literature use activities calculated in the absence of an electrolyte and of an applied potential [1]. The reactivity descriptor is the binding energy $E_{M\text{-}O2}$ of dioxygen to the active site (metal center in. metal complexes) Other volcano correlations compare catalytic activity as the exchange currents *io versus* $E_{M\text{-}O2}$ Even though these correlations predict the most active catalyst, the conditions are far removed from real or operando conditions [2] where the O_2 cathode is far removed from the equilibrium potential. The volcano correlations show [3-6] that perfluorinated Fe phthalocyanine 16(F)FePc) is the most active catalyst and exhibits the largest activation energy!!!. In contrast, the case of biomimetic Fe porphyrins, even though they appear in the low portion of the volcano. In living systems, these complexes are highly active in ORR; see, for example, cytochrome c [7], an iron porphyrin. The reason for their low activity is that at the operating potentials, they are inactive Fe(III)OH in alkaline media and Fe(III)H_2O in acid [5]. The Fe(III) is inactive for ORR as well as other metals in the (III) state located on the descending region of the volcano [4]. They exhibit strong O_2 binding energies, which facilitate e-transfer to the bound O_2. So essentially the descending region of the volcano is attributed to a gradual loss of Fe(II) active sites [4,5]. This is also true for Mn and Cr complexes, but they have low or even negative activation energies [this work]. In a fuel cell, this cannot be avoided. If the electrode is polarized at very negative potentials, this will release M(II) active species, but the hydrogen electrode does not provide enough free energy for this. Li and Na are more promising anodes for air batteries.

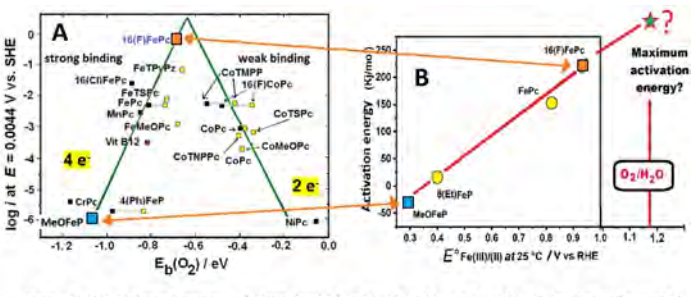


Figure 1. A) Activity volcano correlations for ORR in 0.1 M NaOH. on MN4/graphite electrodes and B) Activation energiees for 4 complexes.

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REFERENCES

1. J.K. Nørskov, J. Rossmeisl, A. Logadottir, L. Lindqvist, J.R. Kitchin, T. Bligaard, ... *J. Phys, Chem*., B 108 (2004) 17886.
2. P. Quaino, F. Juarez, E Santos, W. Schmickler, *Beilstein J. Nanotech.*, 5 (2014) 846
3. L. Scarpetta-Pizo, I. Ponce, R. Oñate, S. del Valle, José H. Zagal, *J. Porphyrins Phthalocyanines* 29, (2025) 304-321
4. J.H. Zagal, M.K.T. Koper *Angew. Chem., Int- Ed.* 55 (2016) 14510-14521,
5. J. H. Zagal, S. Specchia, P. Atanassov, "*Current Op. Electrochem.*, 27, 2021, 100687.
6. T. Burschstein, Y. Yasman, L. Muñoz, J. H. Zagal**,** D. Eisenberg, *ACS Catalysis,* 14,(2024) 22R, Boulatov in "N4 Macrocyclic Metal Complexes**"** J.H. Zagal, F. Bedioui, J.P. Dodelet (Eds) Springer New York (2006)

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Molecular Design Principles of Porphyrinoid-Based Dyes for Efficient Solar Energy Conversion

Tomohiro Higashino[a]

[a]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University*

Dye-sensitized solar cells (DSSCs) have attracted considerable attention due to their potential advantages in terms of power conversion efficiency (PCE), low production cost, design flexibility, and applicability to indoor use. DSSCs are composed of a dye-sensitized TiO_2, a counter electrode, and an electrolyte containing redox shuttles. Based on the fundamental mechanism of photocurrent generation in DSSCs, the overall device performance is strongly governed by the molecular characteristics of the sensitizers and redox shuttles, which play crucial roles in light harvesting and electron transfer processes.[1] Among various organic chromophores, porphyrins and related porphyrinoids have emerged as particularly attractive sensitizers because of their strong visible–near-infrared absorption, rich redox chemistry, and exceptional structural tunability. We aim to establish clear structure–property–performance relationships in porphyrinoid-based DSSCs by exploiting the rich molecular design flexibility of porphyrins, combined with synthetic chemistry, detailed spectroscopic analysis, and systematic evaluation of photovoltaic performance.

For example, we revisited rational molecular design strategies of fused porphyrin dyes as sensitizers for high-performance DSSCs. In principle, the introduction of aromatic-fused structures into porphyrin cores is a promising strategy because direct π-expansion enhances light-harvesting properties. However, fused porphyrin dyes have generally exhibited limited PCEs, which were attributed to unfavorable energy-level alignment, strong molecular aggregation, and shortened excited-state lifetimes. To overcome these challenges, we established a methylene-bridged fusion strategy, which enabled us to surpass the conventional performance limits of fused porphyrin dyes.[2]

We further demonstrate that rational molecular design enables precise control of electron transfer processes in porphyrinoid-based DSSCs.[3] In particular, energy-level engineering of both porphyrin dyes and copper(I/II) redox shuttles allowed us to optimize the driving force for dye regeneration and boost PCEs in porphyrinoid-based DSSCs, clearly demonstrating how molecular-level design of electron-transfer pathways translates into high photovoltaic performance.[4]

In this lecture, I will present our efforts in porphyrinoid-based DSSCs and molecular design of efficient solar energy conversion systems.

REFERENCES

1. T. Higashino, H. Imahori, *Dalton Trans.* **2015**, *44*, 448; Y. Zhang, T. Higashino, H. Imahori, *J. Mater. Chem. A* **2023**, *11*, 12659; T. Higashino, H. Imahori, *ACS Energy Lett.* **2022**, *7*, 1926.
2. Y. Kurumisawa, T. Higashino, S. Nimura, Y. Tsuji, H. Iiyama, H. Imahori, *J. Am. Chem. Soc.* **2019**, *141*, 9910; Y. Zhang, T. Higashino, I. Nishimura, H. Imahori, *ACS Appl. Mater. Interfaces* **2024**, *16*, 67761.
3. Guo, Q.; Higashino, T.; Adachi, R.; Wechwithayakhlung, C.; Packwood, D.; Yamakata, A.; Imahori, H. *ChemSusChem* **2024**, *17*, e202301661.
4. Zhang, Y.; Higashino, T.; Namikawa, K.; Osterloh, W. R.; Imahori, H. *Chem. Sci.* **2025**, *16*, 15004.

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AWARDS

Porphyrinoids as a Molecular Platform for Revealing and Understanding Excited-State Aromaticity

Juwon Oh

Department of Chemistry and Green-Nano Material Research Center, Kyungpook National University, Daegu 41566, Korea

The concept of aromaticity has long served as a central framework for understanding the stability, electronic structure, and reactivity of π-conjugated molecules. Among aromatic systems, porphyrinoids have played a particularly important role in the development of aromaticity concepts, as they represent prototypical macrocyclic molecules that exhibit pronounced global aromaticity beyond local aromaticity at individual pyrrole units.[1] These distinctive features have made porphyrinoids indispensable in advancing our understanding of aromaticity in extended π-systems.

Beyond ground-state aromaticity, Baird's rule predicts a reversal of Hückel aromaticity and antiaromaticity upon electronic excitation.[2] Despite its conceptual importance, however, direct experimental validation and practical utilization of excited-state aromaticity remained elusive for several decades. Here, it will be highlighted how porphyrinoids have emerged as a uniquely powerful molecular platform for the experimental verification, mechanistic understanding, and functional exploration of excited-state aromaticity and antiaromaticity.[3] Owing to their structurally tunable macrocyclic π-systems and the pronounced sensitivity of their electronic structures to (anti)aromatic character, porphyrinoids enable direct spectroscopic observation of aromaticity reversal in excited states.

Through a combination of advanced time-resolved spectroscopies and quantum-chemical calculations, clear experimental signatures of Baird aromaticity and antiaromaticity have been identified across a wide range of expanded and contracted porphyrinoid systems.[4] Beyond conceptual validation, these studies reveal that excited-state aromaticity plays a decisive role in governing photophysical pathways, charge-transfer dynamics, and photochemical reactivity. By establishing design principles that link excited-state aromaticity to controllable molecular function, these findings open new avenues for tuning photoactive π-conjugated systems and developing advanced functional materials. Overall, this presentation aims to illustrate how studies on porphyrinoids contribute to addressing a long-standing fundamental question in excited-state aromaticity and provide useful insights into its effect on excited-state processes.

REFERENCES

1. Y. M. Sung, J. Oh, Y. Cha, W. Kim, J. M. Lim, M. C. Yoon, D. Kim, *Chem. Rev.* **2017**, *117*, 2257-2312.
2. N. C. Baird, *J. Am. Chem. Soc.*, **1972**, *94*, 4941–4948
3. J. Kim, J. Oh, A. Osuka, D. Kim, *Chem. Soc. Rev.*, **2022**, *51*, 268–292.
4. J. Oh, Y. M. Sung, Y. Hong, D, Kim, *Acc. Chem. Res.*, **2018**, *51*, 1349-1358.

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Phthalocyanines as Multifunctional Platforms: Fundamental Electronic Structure, Energy Storage, and Electrocatalytic Applications

Brendon J. McNicholas[a]

[a]*Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37996, United States.*

Phthalocyanines are important building blocks for materials for a variety of energy storage and electrocatalytic applications. My group's research is focused on the fundamental understanding of electronic structure of phthalocyanines and other porphyrinoid macrocycles and their applications in energy storage and electrocatalysis. In my talk, I will focus on three major areas: 1st row transition metal phthalocyanines and substitutions affecting charge-transfer and ligand-centered electronic transitions, main-group phthalocyanines and their applications in semi-solid redox flow batteries, and 1st row transition metal phthalocyanines and substitutions affecting activity for electrocatalytic applications, specifically CO_2 reduction and other small molecule reactions.

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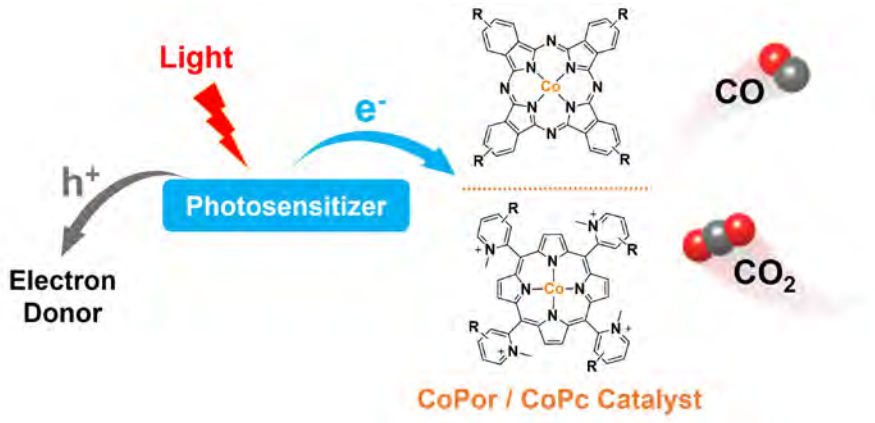
AWARDS

Cobalt Porphyrin or Phthalocyanine Catalysts for CO_2 Photoreduction

Jia-Wei Wang[a], Fan Ma[a]

[a]*School of Chemical Engineering and Technology, Sun Yat-sen University, Zhuhai 519082*

The reduction of CO_2 into chemical feedstocks is a promising means to alleviate the global warming, which is also an indispensable unit in the realization of man-made carbon capture and recycling. To effectively circumvent the multiple possibilities of products and the inertness of CO_2, suitable catalysts are requested for CO_2 reduction to improve the product selectivity and also to drive the reaction at a fast rate. Molecular catalysts, mainly transition metal complexes, continue to attract attention for their well-defined molecular structures and rich redox properties, which are amenable to the rational synthetic optimizations, the isolation of catalytic intermediates and the theoretical analysis on the mechanisms. The use of earth-abundant metals to replace the precious 4d and 5d transition metals is also very appealing to lower the preparation cost and enable the large-scale applications. In this context, it is desirable to exploit effective strategies to design and optimize the earth-abundant molecular catalysts for CO_2 photoreduction [1]. Alternatively, our group has made efforts in designing cobalt porphyrin and phthalocyanine catalysts for CO_2 photoreduction in both homogeneous and hetereogeneous systems [2], along with the investigations on their structure-activity relationship.



REFERENCES

[1] (a) Ma, F.; Luo, Z.-M.; **Wang, J.-W.***, et al. *Coord. Chem. Rev.* 2024, 500, 215529; (b) **Wang, J.-W.***; Ouyang, G. *Acc. Chem. Res.* 2025, 58, 2862-2874.

[2] (a) **Wang, J.-W.**; Jiang, L.; Huang, H. H., et al. *Nat. Commun.* 2021, 12, 4276; (b) Li, Z.; **Wang, J.-W.***; Huang, Y., et al. *Chin. J. Catal.* 2023, 49, 160-167; (c) **Wang, J.-W.***; Zhang, X.; Velasco, L., et al. *JACS Au* 2023, 3, 1984-1997; (d) Ma, F.; Lin, H.-W.; **Wang, J.-W.***, et al. *Molecules* 2024, 29, 4994; (e) **Wang, J.-W.***; Zhao, F.; Velasco, L., et al. *Nat. Commun.* 2024, 15, 9779; (f) Zhao, J. S.; Mu, Y. F.; **Wang, J.-W.***, et al. *Angew. Chem. Int. Ed.* 2024, 63, e202401344.

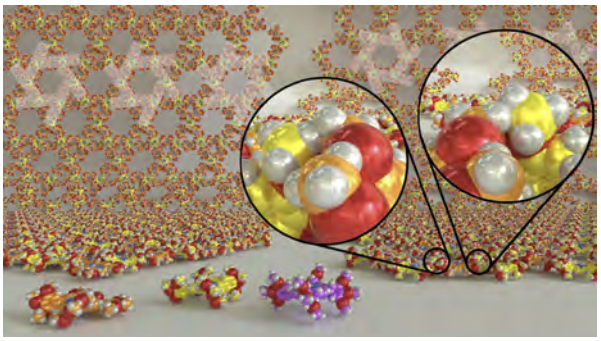
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Conformational diversity in the supramolecular assembly of porphyrins on single crystal substrates

Aisha Ahsan[a], S. Fatemeh Mousavi[a], Aaron Oechsle[b], Narmadha Devi[a], Luiza Buimaga-Iarinca[c], Cristian Morari[c], Thomas A. Jung[b] & Jonathan P. Hill[d]

[a]*University of Basel Switzerland*
[b]*Paul Scherrer Institute Switzerland*
[c]*NIRDIMT Cluj-Napoca, Romania*
[d]*National Institute for Materials Science, Tsukuba, Japan*



Here, we discuss an exceptionally complex on-surface network that forms spontaneously from a single porphyrin module taking up multiple site-specific conformations. We investigate different physicochemical interactions at surfaces that contribute to the symmetry breaking of the porphyrin in its conformational flexion. We compare the binding motifs observed in 3D crystal structures obtained from X-ray diffraction with high-resolution scanning tunneling microscopy and spectroscopy (STM/STS) data and chemical information from X-ray photoelectron spectroscopy (XPS). Density functional theory of the molecular modules on different substrates indicates that the complex interplay of multiple interactions and molecular flexibility is responsible for the observed complexity: Molecular conformational flexibility facilitates the site-specific adaptation of the molecule and its relocation to the most energetically favourable site on the corrugated surface potential [1]. Further, the molecule interacts with the surface-state electrons of the underlying substrate and, via intermolecular hydrogen-bonding, links molecular units at different elevations above the substrate surface. Also, the molecule exhibits conformational diversity across different surface facets of Au(111) [2]. In conclusion, we discuss surfaces and interfaces as possible causes of the emergence of quasi-degeneracy in molecular configurations of supramolecular self-assemblies. The adsorbate-adsorbent interface is recognized as the driver of this system's counterintuitive behavior relative to equilibrium thermodynamics [3].

REFERENCES

1. Mousavi, S. F. *et al*., Communication Chemistry. **8** article number 214 (2025)
2. Baklanov A. *et al.,* J. Am. Chem. Soc., **142**, 1871−1881, (2020)
3. Ahsan, A. *et al*., J. Phys. Chem. Lett. **13**, 7504 –7513 (2022)

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Supramolecular and Materials Sciences with Porphyrins and Phthalocyanines

Takuzo AIDA[a, b]

[a]*Reken Center of Emergent Matter Science, 2-1, Hirosawa, Wako 351-0198, Japan.*
[b]*The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

Porphyrins and phthalocyanines are key functional molecular platforms owing to their rich electronic structures, coordination chemistry, and hierarchical self-assembly. In this lecture, I will present two conceptually related topics that demonstrate how these chemical motifs are utilized for supramolecular chemistry and materials sciences.

First, I introduce solvent-free autocatalytic supramolecular polymerization (SF-ASP) as a template-assisted supramolecular reaction that couples molecular assembly with chemical conversion. Under solvent-free conditions, phthalonitrile precursors are transformed into phthalocyanines through a self-templated process in which the product assembles into ordered supramolecular fibers that promote further reaction. This inhibition-free, termination-free growth resembles living supramolecular polymerization and enables efficient formation of phthalocyanine and metallophthalocyanine assemblies, as well as multistep synthesis of sequence-controlled supramolecular copolymers. SF-ASP thus exemplifies how chemical reactivity can emerge from supramolecular order in a sustainable manner [1].

In the second part, I report a particular porphyrin-based assembly in which conformationally flexible spiral units function as molecular springs, imparting elastic behavior of the assembly under compressive stress. Mechanical deformation induces a cooperative reorganization of supramolecular chirality and packing that minimizes unfavorable intermolecular interactions at the expense of entropy, while release of stress restores the original entropy-favored structure. This behavior demonstrates how entropic modulation within ordered supramolecular assemblies can be translated into reversible mechanical function [2].

Together, these studies highlight how supramolecular polymerization and entropy-driven structural reorganization enable adaptive porphyrin- and phthalocyanine-based systems that integrate sustainable synthesis, structural precision, and mechanical responsiveness.

REFERENCES

1. Z. Chen et al., *Nat Mater.* **2022**, *21*, 253–261.
2. W. Yuan, H. Sato *et al.*, submitted.

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Star-Shaped Polymers with a Phthalocyanine Core for Organic Memory Devices

Junko Aimi[a]

[a]*National Institute for Materials Science (NIMS), Japan*

ORALS

Topological polymers such as block copolymers, branched polymers, and star polymers, exhibit unique three-dimensional microstructures in bulk, thin films, or solutions. Incorporating functional molecules into such polymer microstructures presents various applications in materials science. For instance, polymeric materials containing π-extended aromatic compounds including porphyrins and metallo-phthalocyanines (MPc) have been synthetic targets for practical applications in organic electronics, because they show outstanding photochemical and electronic properties.

We have prepared star-shaped polymers with an MPc core and applied them to organic field-effect transistor (OFET) memory devices. Non-volatile OFET memory presents a promising technology for wearable data storage due to its non-destructive read-out memory cell system, multi-bit storage capability, and easily integrated structure. In these devices, the memory layer resides between the organic semiconductors and control gates, storing and releasing charges during the writing and erasing processes. The star-shaped polymer with an MPc functions like a nano-floating gate, capable of storing and releasing hole charges. Also, its polystyrene arms form homogeneous polymer films and inhibit leakage of the trapped charges. A bottom-gate top-contact OFET memory device, utilizing pentacene as the organic semiconductor and MPc-cored star polymer (MSP) as the memory layer, demonstrated flash-type memory characteristics with a high memory on/off current ratio of 10^7, long retention ability, and good endurance.[1] The memory device performance, including memory window and charge retention time, can be controlled by tailoring star polymer design through precision polymer synthesis.[2][3] In addition, the OFET memory can be fabricated via a one-pot solution process via polymer-matrix assisted phase separation of MSP and a soluble organic semiconductor.[4] The star-shaped polymer was easily fabricated in logic circuits such as inverters, demonstrating multilevel or reconfiguarable logic-in-memory applications.[5][6][7] The star-shaped polymer nano-floating gate is a promising material to prepare high-performance OFET memory devices and is useful for integrating flexible organic devices and large-area memory devices. The preparation and device performance of the OFET memory with polymer nano-floating gate will be discussed.

REFERENCES

1. J. Aimi, C. T. Lo, H. C. Wu, C. F. Huang, T. Nakanishi, M. Takeuchi, W. C. Chen, *Adv. Electron. Mater.*, **2016**, *2*, 1500300.
2. J. Aimi, P. H. Wang, C. C. Shih, C. F. Huang, T. Nakanishi, M. Takeuchi, H. Y. Hsueh, W. C. Chen, *J. Mater. Chem. C*. **2018**, *6*, 2724.
3. X. Zhong, D. Panigrahi, R. Hayakawa, Y. Wakayama, K. Harano, M. Takeuchi, J. Aimi, *J. Mater. Chem. C,* **2024**, *12*, 9642.
4. J. Aimi, T. Yasuda, C. F. Huang, M. Yoshio, W. C. Chen, *Mater. Adv.*, **2022**, *3*, 3128.
5. D. Panigrahi, R. Hayakawa, X. Zhong, J. Aimi, Y. Wakayama, *Nano Lett*, **2023**, *23*, 319.
6. R. Hayakawa, X. Zhong, K. Honma, D. Panigrahi, J. Aimi, K. Kanai, Y. Wakayama, *Nano Lett,* **2023***, 23,* 8339.
7. Y. Shingaya, T. Iwasaki, R. Hayakawa, S. Nakaharai, K. Watanabe, T. Taniguchi, J. Aimi, Y. Wakayama, *ACS Appl. Mater. Interfaces,* **2024***, 16*, 33796.

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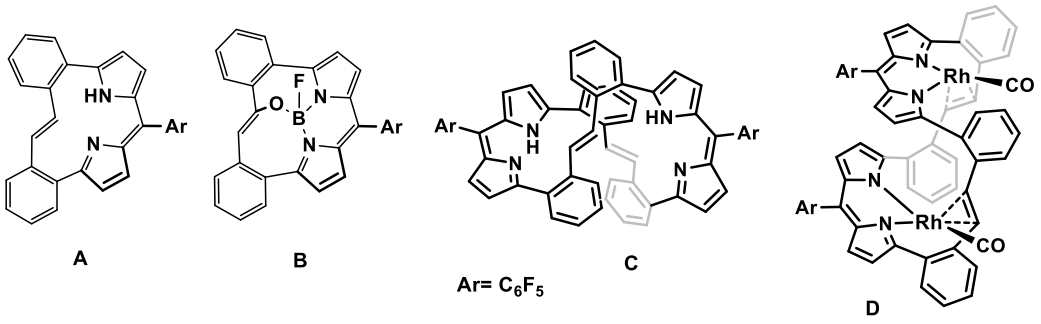
Meso-Modified Porphyrinoids: Its B(III) and bis-Rh(I) Complexes

A. Srinivasan[a], Rampal Vishwakarma,[a] Mainak Das[b]

[a]*School of Chemical Sciences, National Institute of Science Education and Research (NISER), An OCC of Homi Bhabha National Institute, Bhubaneswar 752050, Odisha (India).*
[b]*Sorbonne Université, CNRS, Institut Parisien de Chimie Moléculaire, IPCM, Paris 75005, France.*

ORALS

Modifying the number or configuration of *meso*-carbons in the porphyrin core alters the steric environment and electronic delocalization within the macrocycle. By decreasing or increasing the number of *meso*-carbons or heterocyclic rings in the tetrapyrrolic core led to the formation of contracted or expanded porphyrinoids.[1] To achieve such modified analogues, as a strategy, (i) *meso*-carbon appended with *ortho*-benzannulation at the periphery of the core for rigidity and (ii) vinylogous linkages for flexibility are introduced. In the first part, we wish to highlight the synthesis of *E*-stilbene imprinted cyclic diphyrin (**A**). The vinylene or ethylene twist in **A** disrupts global conjugation while preserving the local aromaticity, thus introducing a new class of contracted porphyrinoid with non-aromaticity. Complexation of **A** with B(III) ion generates asymmetric ring formation within the cavity and transformation of non-emissive diphyrin into emissive in solution (**B**).[2] At the end, we demonstrate the synthesis of porphyrin resembling macrocycles, where the design enables stimuli-responsive conformational plasticity and tunable (anti)aromaticity, manifesting as moderate Hückel antiaromaticity in freebase (**C**), weak Möbius aromaticity upon protonation, and nonaromaticity through bis-Rh(I) complexation (**D**), resulting in foldameric structures with η^2 coordination and panchromatic absorption.[3] Overall, the strategy reveals topology−property relationships in π-conjugated macrocycles.



REFERENCES

1. a) T. D. Lash, *Chem. Rev*. **2017**, *117*, 2313-2446; b) B. Szyszko, L. Latos-Grażyński, *Angew. Chem. Int. Ed.* **2020**, *59*, 16874-16901 ; c) M. Das, B. Adinarayana, A. Srinivasan, *ACS Omega* **2021**, *6*, 35204-35212.
2. R. Vishwakarma, D. Blasco, D. Sundholm, N. Ch. Jana, M. Das, A. Srinivasan, *Org. Lett*., **2025**, *27*, 6429-6433.
3. R. Vishwakarma, M. Das, A. Srinivasan, *Inorg. Chem.*, **2026**, *65*, 149-155.

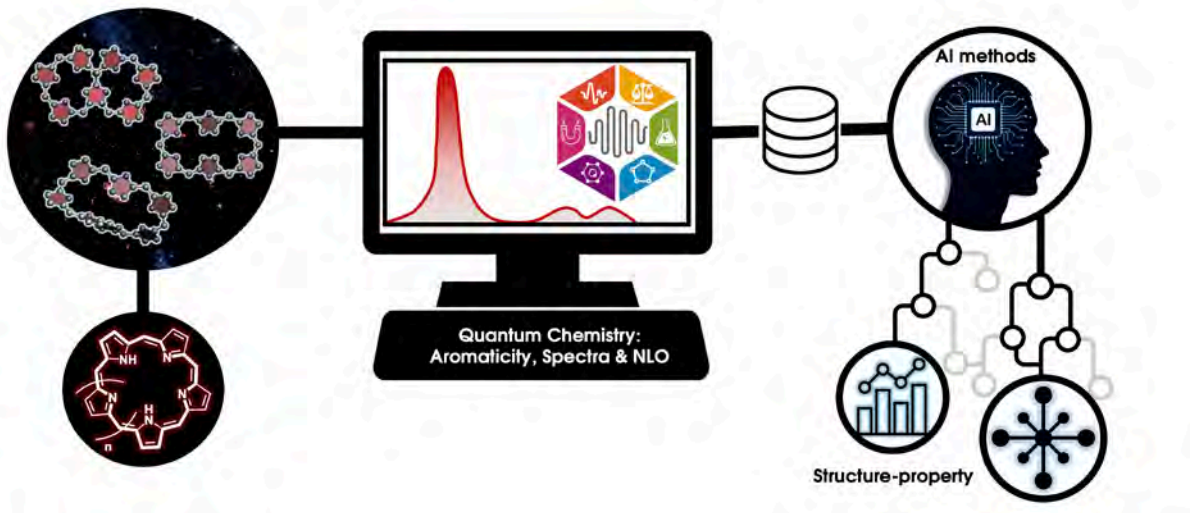
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Aromaticity in the Spectroscopic Spotlight: Expanded Porphyrins

Mercedes Alonso[a], **Eline Desmedt**[a], **F. De Vleeschouwer**[a]

[a] *General Chemistry Research Group, Algemene Chemie (ALGC), Vrije Universiteit Brussel, 1050 Brussel, Belgium*

Spectroscopic observables are widely used to infer ground- and excited-state aromaticity in expanded porphyrins. However, how reliably these photophysical signatures reflect aromaticity across chemically diverse systems remains an open question. In this talk, I will examine a broad family of hexaphyrins spanning different redox states, topologies, peripheral substitutions, and core modifications, and ask whether commonly assumed spectroscopic markers of aromaticity remain valid. By combining TD-DFT calculations with multiple aromaticity descriptors and chemical compound space analyses, we uncover a subtle interplay between molecular planarity, electronic structure, aromaticity, and absorption spectra [1]. Notably, our results demonstrate that the general assumption that *antiaromatic expanded porphyrins exhibit significantly attenuated absorption bands compared to aromatic counterparts* should be applied with caution. Then, I will turn to nonlinear optical (NLO) properties and illustrate how explainable artificial intelligence can be used to disentangle the key factors governing the NLO response of hexaphyrins [2]. In particular, we address the central question: which structural and electronic features control NLO activity in these systems? Overall, these findings underscore the need for a multidimensional approach to quantify aromaticity in porphyrinoid macrocycles, going beyond spectroscopic observables alone, with innovative computational and data-driven strategies emerging as powerful tools for uncovering robust structure–property relationships across chemical compound space [3].



REFERENCES

1. E. Desmedt, I. Casademont-Reig, R. Monreal-Corona, F. De Vleeschouwer, M. Alonso, *Chem. Eur. J.* **2024**, *30*, e202401933.
2. E. Desmedt, M. Jacobs, M. Alonso, F. De Vleeschouwer, *Phys. Chem. Chem. Phys.* **2025**, *27*, 1256.
3. F. De Vleeschouwer, E. Desmedt, M. Alonso, M. *Chem. Methods* **2025**, *5*, e202500064.

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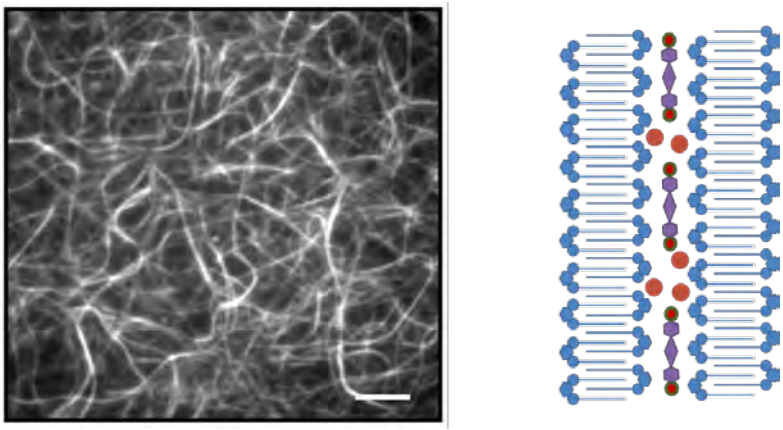


Antimicrobial behaviour of supramolecular gels containing a variety of porphyrins

David B Amabilino[a], Kavya Anguluri[b,c], Bunty Sharma[d], Saman Bagherpour[b,c], Ana C Calpena[c,e], Lyda Halbaut[e], Gurpreet Kaur[f], Ganga Ram Chaudhary[d,f], Lluïsa Pérez-García[b,c]

[a]*Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Carrer dels Til.lers, Bellaterra, Spain*
[b]*Departament de Farmacologia, Toxicologia i Química Terapèutica, Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, Spain*
[c]*Institut de Nanociència i Nanotecnologia IN2UB, Universitat de Barcelona, Barcelona, Spain*
[d]*Department of SAIF/CIL, Panjab University, Chandigarh, India*
[e]*Departament de Farmàcia, Tecnologia Farmacèutica, i Fisicoquímica,, Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, Spain*
[e]*Department of Chemistry and Centre of Advanced Studies in Chemistry, Panjab University, Chandigarh, India*

The use of encapsulation of a family of tetraphenylporphyrins in a supramolecular gel formed using a bis-imidazolium-based provides materials that generate singlet oxygen upon light excitation. The gels comprise fibres that incorporate one of the four porphyrins: 5,10,15,20-tetrakis(*N*-methyl-4-pyridinium)porphyrin tetraiodide, 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin, 5,10,15,20-tetrakis(3-hydroxyphenyl)porphyrin) or 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin. The porphyrins are trapped in the fibres (see image below).



All thee gels are viscoelastic, suggesting their potential as manipulable delivery systems that can retain their gel form.[1] The singlet oxygen generation from the hydrogel matrix is higher than solutions of the chromophores, as seen before by us.[2] The generation of the singlet oxygen was screened as a way to attain antimicrobial activity. The pyridinium-derived porphyrin-containing gel had the highest reduction in E. coli and S. aureus colony forming, indicating their promise in antimicrobial photodynamic treatments.

REFERENCES

1. K. Anguluri, B. Sharma, S. Bagherpour, A.C. Calpena, L. Halbaut, D. B. Amabilino, G. Kaur, G. R. Chaudhary, L. Pérez-García, *Photodiagnosis Photodyn. Ther.*, 2025, **52**, 104529.
2. M. Samperi, D. Limón, D.B. Amabilino, L. Pérez-García, *Cell Rep. Phys. Sci*., 2020, **1**, 100030.

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Medicinal precursor synthesis from carbon dioxide with zinc porphyrin/ATP-NADH dependent biocatalysts hybrid system

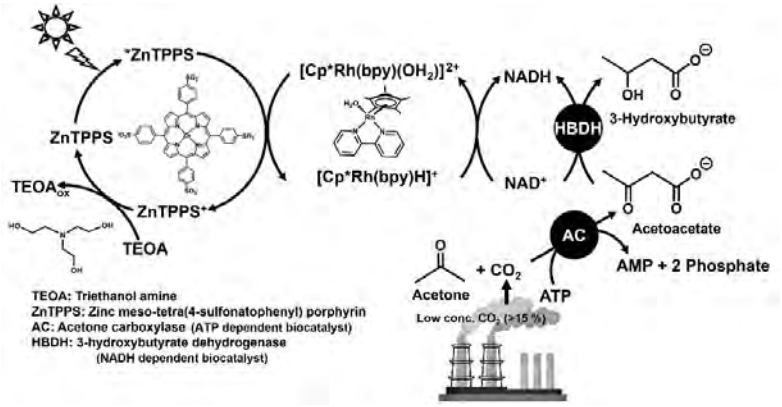
Yutaka Amao[a,b]

[a] *Graduate School of Science, Osaka Metropolitan University, 3-3-138, Sugimoto, Sumiyoshi-ku, Osaka, 558-8585 Japan*
[b] *Research Centre for Artificial Photosynthesis, Osaka Metropolitan University, 3-3-138, Sugimoto, Sumiyoshi-ku, Osaka, 558-8585 Japan*

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A novel medicinal precursor, 3-hydroxybutyrate synthesis from gaseous CO_2 and acetone using a visible-light driven hybrid catalytic system consisting of triethanol amine (TEOA), water-soluble zinc porphyrin, zinc tetraphenylporphyirn tetrasulfonate (ZnTPPS), $[Cp^*Rh(bpy)(H_2O)]^{2+}$(Cp^*: 1,2,3,4,5-pentamethylcyclopentadien, bpy: 2,2'-bipyridine), $NAD^{+,}$ and various biocatalysts is a candidate for a useful method as a green process. In this presentation, an enzyme extract containing ATP dependent acetone carboxylase (AC) and NADH dependent 3-hydroxybutyrate dehydrogenase (HBDH) from culturing a purple nonsulfur photosynthetic bacterium, *Rhodobacter capsulatus* in a medium containing acetone and bicarbonate under anaerobic photoheterotrophic conditions was applied as a catalyst for the visible light-driven 3-hydroxybutyrate synthesis from acetone and gaseous CO_2 system of TEOA, ZnTPPS, $[Cp^*Rh(bpy)(H_2O)]^{2+}$and NAD^+ in the presence of ATP was introduced as an example for a medicinal precursor production from low concentration of gaseous CO_2 (>15 %) with the zinc porphyrin/ ATP-NADH dependent biocatalytic system as shown in Figure 1[1-4].

Fig. 1. Visible-light-driven 3-hydroxybutyrate synthesis from acetone and low concentration CO_2 with the combination of NAD^+ reduction system of TEOA as an electron donor, ZnTPPS as a photosensitizer, $[Cp^*Rh(bpy)(H_2O)]^{2+}$, and biocatalysts (AC and HBDH) in the presence of ATP.



REFERENCES

1. Y. Kita, Y. Amao, *Chem. Commun.*, 58, 11131 (2022).
2. Y. Kita, R. Fujii, Y. Amao, *Sustain. Energy Fuels*, 7, 360 (2023).
3. Y. Kita, Y. Amao, *Bull. Chem. Soc. Jpn.,* 96, 328 (2023).
4. Y. Kita, Y. Amao, *Green Chem.,* 25, 2699 (2023).

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Advances in Photodynamic Materials for Antimicrobial and Environmental Applications

Amuhaya E. K.[a], Isaiah B. M.[a,b], Murage M.W.[a,c], Nyokong T.[d]

[a]*United States International University – Africa, Nairobi, Kenya*
[b]*Technical University of Kenya, Nairobi, Kenya*
[c]*University of Nairobi, Nairobi, Kenya*
[d]*Rhodes University, Makhanda, South Africa*

ORALS

Recent research in our group has focused on the design and development of photochemically active materials to address persistent microbial and environmental challenges. Central to this work is the synthesis, modification, and photophysical characterization of porphyrin-based photosensitizers with enhanced performance under visible-light irradiation. Systematic structural tuning of phenolic and cationic porphyrins has enabled the establishment of clear structure–property relationships governing light absorption, intersystem crossing, triplet-state lifetimes, and singlet oxygen generation. These findings have supported the rational development of photosensitizers with improved stability and photodynamic efficiency.

Parallel efforts have focused on incorporating these optimized photosensitizers into polymer-supported systems, notably polysulfone nanofibers and related composite membranes [1]. These materials were engineered to enhance photosensitizer retention, promote water compatibility, and improve long-term operational stability. Antimicrobial evaluations performed under illuminated and dark conditions have demonstrated substantial photodynamic inactivation of waterborne pathogens, along with favourable reusability and material robustness. These results highlight the potential of light-driven antimicrobial materials for practical water treatment applications.

In addition to antimicrobial performance, this research has explored broader environmental photochemistry themes, including the behaviour of reactive oxygen species, light-driven degradation pathways, and the operational feasibility of photodynamic systems in low-resource contexts. Collectively, these investigations underscore the promise of photosensitizer-integrated materials as sustainable, adaptable solutions for improving water quality and advancing environmental health [2, 3].

REFERENCES

1. Isaiah B.M, Amuhaya E.K, Muhanji C.I, Sindelo A., Nyokong, T., Smith G.S. Photosensitizer formulations based on porphyrins and zinc oxide nanoparticles for water treatment. *Journal of Porphyrins and Phthalocyanines* 0 0:0, A-N
2. Murage M.W, Amuhaya E.K, Mbatia B.N, Muge E.K, Enhanced Antifungal Efficacy of Porphyrin-Mediated 1 Photodynamic Therapy Synergistically Combined with 2 Fluconazole Against Candida *spp. Journal of Porphyrins and Phthalocyanines* **2025** 29:07, 792-806
3. Murage M.W., Amuhaya E.K., Mbatia B.N, Muge E.K., and Derese S. Synergistic effect of porphyrin-induced photodynamic antimicrobial chemotherapy combined with Gentamicin against clinically important gram-positive and gram-negative bacteria. *Journal of Porphyrins and Phthalocyanines* **2024** 28:11n12, 814-829

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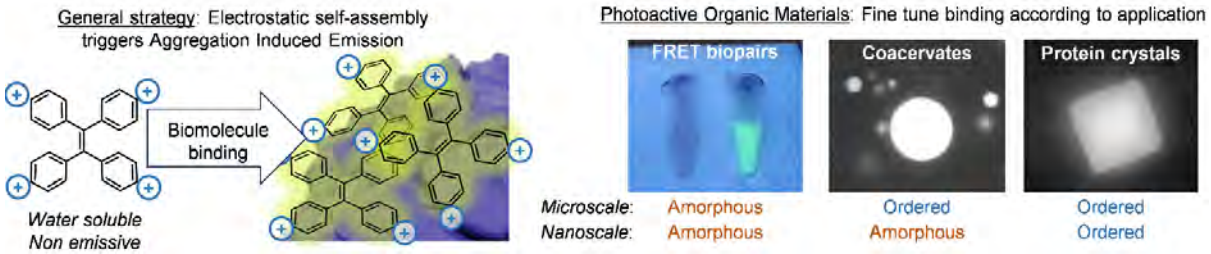
Multifaceted exploration of aggregation in water: from self-assembly to liquid-liquid phase separation

Alba Sanz-Velasco[a], Prof. Eduardo Anaya-Plaza[a,b]

[a] *Faculty of Medicine and Health Technology. Korkeakoulunkatu 1, FI-33014 Tampere University*
[b]*Department of Bioproducts and Biosystems, School of Chemical Engineering, Aalto University. Kemistintie 1, Espoo, Finland. eduardo.anaya(at)aalto.fi*

ORALS

Molecular materials like phthalocyanines have numerous applications in biotechnology, including their use as imaging agents, photosensitizers for photodynamic therapy, and as biomaterials. However, similar to most fluorophores, phthalocyanines face a key challenge in aqueous media: their hydrophobic nature lead to aggregate and precipitate, resulting in the loss of excited state properties, such as fluorescence.
To address this, we initially developed bioconjugation strategies that utilize the electrostatic self-assembly of phthalocyanines for diverse applications.[1] Nonetheless, there exists a family of compounds known as aggregation-induced emitters (AIEs) that capitalize on their limited solubility in water. In the aggregated state, their molecular vibrations and rotations—which would otherwise deactivate their emission—are restricted, thereby restoring their emissive properties.[2]
Through a carefully tailored chemical design, AIEs can be precisely controlled in their self-assembly,[3] which can lead to the formation of monomerically dissolved molecules, crystalline arrays, or liquid-liquid phase separation (LLPS).[4] The latter is particularly significant in the fields of biomedicine and biotechnology, offering substantial potential for developing biomaterials, such as biohybrid silk fibers and protein crystals.



REFERENCES

(1) Almeida-Marrero, V.; van de Winckel, E.; Anaya-Plaza, E.; Torres, T.; de la Escosura, A. Porphyrinoid biohybrid materials as an emerging toolbox for biomedical light management. *Chem Soc Rev* **2018**, *47* (19), 7369–7400. DOI: 10.1039/c7cs00554g
(2) Wang, H.; Li, Q.; Alam, P.; *et al*. Aggregation-Induced Emission (AIE), Life and Health. *ACS Nano* **2023**, *17* (15), 14347–14405. DOI: 10.1021/acsnano.3c03925
(3) Sanz-Velasco, A.; Amargos-Reyes, O.; Kahari, A.; Lipinski, S.; Cavinato, L. M.; Costa, R. D.; Kostiainen, M. A.; Anaya-Plaza, E. Controlling aggregation-induced emission by supramolecular interactions and colloidal stability in ionic emitters for light-emitting electrochemical cells. *Chem Sci* **2024**, *15* (8), 2755–2762. DOI: 10.1039/d3sc05941c
(4) Tersteegen, J.; Tunn, I.; Sand, M.; Valisalmi, T.; Malkamaki, M.; Gandier, J. A.; Beaune, G.; Sanz-Velasco, A.; Anaya-Plaza, E.; Linder, M. B. Recombinant silk protein condensates show widely different properties depending on the sample background. *J Mater Chem B* **2024**, *12* (46), 11953–11967. DOI: 10.1039/d4tb01422g

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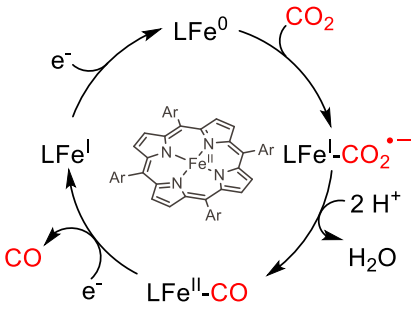
O_2 activation and CO_2 reduction using Mn and Fe porphyrins : operando spectroelectrochemical mechanistic studies

Elodie Anxolabéhère-Mallart, Julien Bonin, Claire Fave, Marc Robert

Sorbonne Université, Institut Parisien de Chimie Moléculaire, CNRS UMR 8232
4 Place Jussieu, 75252 Paris Cedex 05, France
elodie.anxolabehere@sorbonne-universite.fr

ORALS

The development of spectroelectrochemistry (SEC), which integrates spectroscopic and electrochemical techniques, has become a powerful approach for uncovering reaction mechanisms at the molecular scale. SEC offers strong evidence for the presence of reaction intermediates and enables more reliable interpretation of the structures of the species identified. In particular, coupling cyclic voltammetry with infrared (IR) and UV–visible SEC has proven highly valuable for detecting reaction intermediates.
We will show how in situ and operando SEC serves as an essential tool for gaining insight into the activation of small molecules and will illustrate our point with examples related to CO_2 reduction [1,2] and O_2 reductive activation[3,4] using Mn and Fe porphyrins catalysts (scheme 1).
We will describe promising results of electrocatalysis experiments which can lead to new electrosynthesis processes, thus promoting the development of more sustainable and efficient synthetic reactions.



Scheme 1: Proposed catalytic cycle for CO_2 reduction using Fe porphyrin showing successive intermediates reactive species

REFERENCES

1. D. Mendoza, S.-T. Dong, N. Kostopoulos, V. Pinty, O. Rivada-Wheelaghan, E. Anxolabéhère-Mallart, M. Robert, B. Lassalle-Kaiser *ChemCatChem* **2023**, *15*, e202201298.
2. A. Salamé, M. H. Cheah, J. Bonin, M. Robert, E. Anxolabéhère-Mallart Angew. Chem. Int. Ed. **2024**, e202412417.
3. (a) R. Oliveira, W. Zouari, C. Herrero, F. Banse, B. Schöllhorn, C. Fave, E. Anxolabéhère-Mallart *Inorg. Chem*. **2016**, 55, 23, 12204-12210; (b) N. Kostopoulos, C. Achaibou, J.-M. Noël, F. Kanoufi, M. Robert, C. Fave, E. Anxolabéhère-Mallart *Inorg. Chem.* 2020, 59, 11577-11583.
4. N. Kostopoulos, F. Banse, C. Fave, E. Anxolabéhère-Mallart *Chem. Comm*., 2021, 57, 1198-1201.

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Novel Synthetic Method and 22π Global Annulene Aromaticity of Photochromic Dibenzodimethyldihydropyrenes

Naoki Aratani[a], **Hirofumi Morimoto**[a], **and Hiroko Yamada**[b]

[a]*Division of Materials Science, Nara Institute of Science and Technology, 8916-5 Takayama-cho, Ikoma 630-0192, Japan*
[b]*Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*

ORALS

Dibenzo-*m*-cyclophane (**DC**) is a photochromic compound that converts to green dibenzodimethyldihydro-pyrene (**DP**) upon irradiation of UV light, and quickly returns to **DC** at room temperature.[1] We have developed a facile synthetic method of **DC**s using Suzuki-Miyaura cross-coupling reactions, which made the synthetic steps short and facilitated the introduction of various substituents.

In the **DC** state, the number of aromatic units is 6π (benzene) × 4, which results in no absorption in the visible region (colorless) (Figure 1). Irradiation of UV light (365 nm) to the **DC** isomerizes it to a large 22π annulene aromatic system of **DP** with visible-to-near-infrared (NIR) absorption, which was confirmed by experimental evaluation and theoretical calculations (Figure 2). We observed that the half-lifetimes of **DP**s are 0.5–20 sec, depending on the substituents. There is a correlation between the activation barrier from **DP** to **DC** and the half-lifetimes of **DP**s; 2,7-dimethoxy-**DP** has the longest half-life, exceeding 2 minutes. Besides, they can photo-isomerize not only in solution but also in films.

We will report the substituent effects and physical properties of **DC** and **DP**.

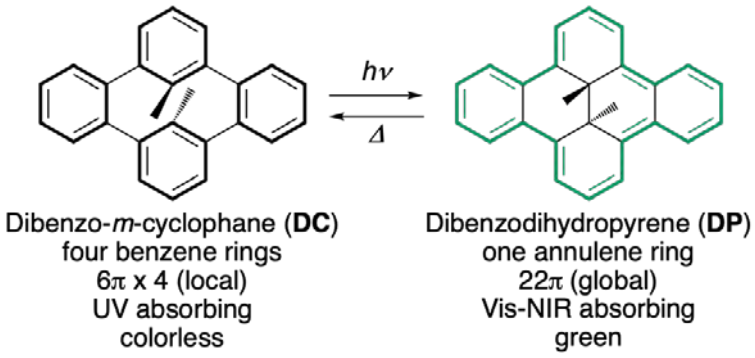


Figure 1. Photochromic reaction between dibenzo-*m*-cyclophane (**DC**) and dibenzodihydro-pyrene (**DP**).

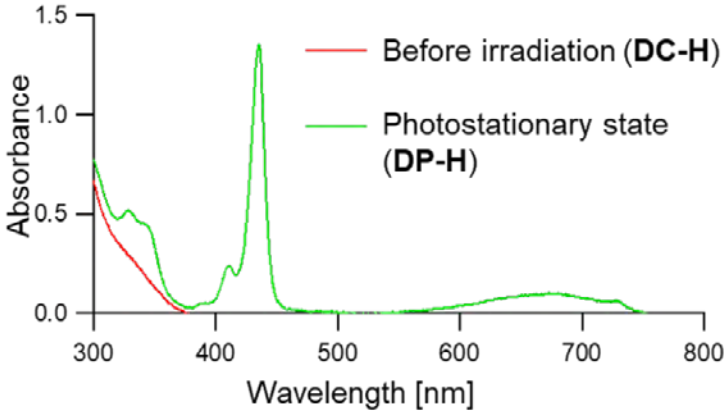


Figure 2. UV-vis absorption spectra of **DC** and **DP** in toluene.

REFERENCES

1. R. H. Mitchell and Y. Chen, *Tetrahedron Lett*. **1996**, *37*, 5239.

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Bacteriochlorins and Phthalocyanins in Photoacoustic Tomography

Luis G. Arnaut[a]

[a]*Chemistry Department, University of Coimbra, 3004-535 Coimbra, Portugal*

ORALS

Photoacoustic tomography (PAT) is a new tool for the armamentarium of noninvasive imaging inside the body. PAT combines the contrast of spectroscopic techniques with the depth of acoustic methods. Although the use of light to excite a chromophore and of ultrasound detection to identify its location, offers new opportunities for imaging, the development of chromophores, or contrast agents, for PAT is still at its infancy. The physical basis for the generation of a photoacoustic wave is a fast (sub-microsecond) volume change. Nanosecond pulsed lasers are employed to excite a chromophore absorbing in the red/near-infrared region of the spectrum and the subsequent radiationless transitions provide thermal energy to launch a thermoelastic expansion. Most often this thermoelastic expansion is at the origin of the photoacoustic wave. In special cases, the heat released is used to promote a phase change, from a nanodroplet to a microbubble, and a larger volume change can be achieved.
This lecture will present PAT of tumors using pulsed lasers and bacteriochlorins with strong absorption at ~750 nm. It will be shown that the signal of the bacteriochlorin can be deconvoluted from those of oxy- and desoxyhemoglobin, to assess the biodistribution of the bacteriochorin in the tumor and surround tissues [1,2]. It will also be shown that phthalocyanines can be associated with nanodroplets of perfluoropentane and when excited at 727 nm provide enough thermal energy to vaporize the nanodroplets and form microbbubles [3]. This process is reversible and repetitively produces high intensity photoacoustic waves.
The challenges and opportunities of PAT using thermoelastic expansion or phase transitions are discussed, and their effect in the tumor microenvironment is investigated.

REFERENCES

1. C. S. Lobo, M. I. P. Mendes, D. A. Pereira, L. C. Gomes-da-Silva, L. G. Arnaut, *Sci. Rep*., 13 (2023) 11667.
2. M. Penetra, B. Lima, J. P. A. Campos, S. M. A. Pinto, F. A Schaberle, M. M. Pereira, L. G. Arnaut, L. C. Gomes-da-Silva, *Angew. Chem*., *Int. Ed.*, (2025) e09121.
3. M. I. P. Mendes, C. D. F. Coelho, F. A. Schaberle, M. J. Moreno, M. J. F. Calvete, L. G. Arnaut,* *RSC Adv.*, 13 (2023) 35040-35049.

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Optical characterisation of single chlorophyll molecules at the sub-nanometre scale

Thiago G. L. Brito*[a], Daniel Arribas*[a], Myriam Wadsack[a], Claudia Leticia Gómez Flores[a], Irena Padniuk[a], Victor Feitosa[a,b], Klaus Kuhnke[a], Klaus Kern[a,c], Kelvin Anggara[a], Anna Rosławska[a]

[a]*Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany*
[b]*University of Campinas - UNICAMP, Campinas 13083-859, Brazil*
[c]*École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland*

As one of the main biomolecules harvesting light in photosynthetic organisms, chlorophyll plays a crucial role in biological systems, ultimately sustaining life on Earth. Therefore, the fundamental understanding of the optical properties of this porphyrin-related biomolecule has attracted widespread interest from the scientific community. However, traditional spectroscopic experiments, often probing complexes, only provide an averaged understanding of the rich photophysics of chlorophyll, where the effects of each possible molecular configuration and the local environment are smeared out. In this work, we address this by exploiting the sub-nm resolution of scanning tunnelling microscopy and the highly-localised plasmonic enhancement of the picocavity at the tunnelling junction. We characterise individual chlorophyll molecules, deposited by electrospray ion beam deposition on a Ag(111) surface with NaCl islands as decoupling layer. By analysing their fluorescence emission excited by the tunnelling electrons or an external laser source and their tip-enhanced Raman spectra, we observe the structural dependency of the molecular opto-electronic properties. Our investigation opens new opportunities for the fundamental understanding of light-harvesting during photosynthesis with unprecedented sub-molecular resolution.

*Equally contributing authors

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On-Surface Reactions for Chain-Like Porphyrin Architectures

Willi Auwärter[a]

[a] *Physics Department E20, TUM School of Natural Sciences, Technical University of Munich, James-Franck-Str. 1, D-85748 Garching, Germany*

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On-surface synthesis protocols provide elegant routes to individual porphyrinoids and tetrapyrrole-based one- (1D) and two-dimensional (2D) nanostructures on coinage metal supports [1-3], including covalent architectures as well as organometallic coordination polymers.
In this presentation, I will focus on two of our recent approaches to create and comprehensively characterize 1D structures from porphyrins in an ultrahigh vacuum environment. First, a halogenated porphyrin equipped with terminal CF_3 groups, provided by the group of Mathias O. Senge (Trinity College, Dublin), is used to probe thermally-induced dehalogenation reactions on Au(111) and Ag(111) supports. After selective activation of the β-position, the porphyrins form different reactions products, including Au- and Ag-coordinated chains. Configuration and electronic properties are characterized with submolecular resolution by scanning tunneling microscopy, spectroscopy and non-contact atomic force microscopy. Second, we aim to extend porphyrin architectures by including non-conjugated rigid hydrocarbon linkers, namely BCP [4,5]. Thermally-induced coupling reactions on Au(111) result in chain-like ribbons. The coupling motifs are discussed based on a scanning probe microscopy characterization. These studies give access to novel surface-supported porphyrinoid structures with distinct chemical and physical properties and shed light on the underlying on-surface reactions.

REFERENCES

1. Deyerling, J. *et al.* J. Phys. Chem. C **2022,** 126, 8467.
2. Corral Rascon, E.; *et al. J. Am. Chem. Soc*. **2023,** *145*, 967.
3. Deyerling, J. *et al.* Angew. Chem. Int. Ed. **2025,** 64, e202412978.
4. Locke, G.M..; *et al. Chem. Eur.J.* **2019,** *25*, 4590.
5. Yang, B..; *et al. Angew. Chem. Int. Ed.* **2023,** *62*, e202218211.

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Metal phthalocyanines and their hybrid structures as active layers of chemiresistive gas sensors

Tamara Basova[a]

[a]*Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia*

The development of novel sensing materials capable of detecting trace toxic gases in ambient air remains a critical scientific and technological challenge. Hybrid architectures combining metal phthalocyanines (MPcs) with carbon nanotubes (CNTs) and noble metal nanoparticles (MNPs) have emerged as highly promising platforms for next-generation chemiresistive sensors.

In this work, we present an overview of our group's recent advances in designing MPc-based active layers for chemiresistive gas sensors, with a primary focus on the sensors for ammonia detection. Among various MPcs, fluoro-substituted derivatives, particularly cobalt and zinc phthalocyanines ($MPcF_x$), exhibit exceptional sensitivity to sub-ppm NH_3 concentrations, with detection limits as low as 0.1 ppm. These thin films were fabricated via physical vapor deposition, enabling precise control over morphology and composition. Systematic studies revealed that both the number and positional arrangement of fluorine substituents on the phthalocyanine macrocycle significantly influence sensor response [1].

Further performance enhancement was achieved through hybridization with single-walled carbon nanotubes (SWCNTs). Non-covalent and covalent functionalization strategies were employed to integrate MPcs with SWCNTs. It was shown that the use pyrene-functionalized phthalocyanines improves the interaction between MPc and SWCNT. Increasing the number of pyrene substituents (from 1 to 4) progressively amplified the NH_3 response, yielding hybrid films with a detection limit of 0.4 ppm [2].

We also explored 3D architectures in which SWCNTs are cross-linked via covalently attached MPc units. Comparative analysis demonstrated that these 3D networks outperform conventional MPc/SWCNT composites in sensor response, highlighting the critical role of nanotube functionalization architecture [3].

Finally, we report on hybrid "MNP/MPc" systems fabricated by sequential gas-phase deposition: MPc layers were prepared by physical vapor deposition, while palladium (Pd) and bimetallic Pd/Au nanoparticles were introduced via metal–organic chemical vapor deposition (MOCVD) [4]. These nanostructured hybrids exhibited enhanced sensitivity and selectivity toward hydrogen, even in the presence of interfering reducing gases and volatile organic compounds.

REFERENCES

1. D. Klyamer, D. Bonegardt, T. Basova, Chemosensors 2021, 9, 133.
2. V. Ivanova, D. Klyamer, P. Krasnov, E. N. Kaya, İ. Kulu, S. Tuncel Kostakoglu, M. Durmuş, T. Basova, Sensors Actuators B 2023, 375, 132843.
3. V. Ivanova, A. Şenocak, D. Klyamer, E. Demirbas, S. Makhseed, P. Krasnov, T. Basova, M. Durmuş, Sensors Actuators B: Chemical. 2024, 398, 134733.
4. N.S. Nikolaeva, D.D. Klyamer, S.M. Zharkov, A.R. Tsygankova, A.S. Sukhikh, N.B. Morozova, T.V. Basova, Int. J. Hydrogen Energy 2021, 46, 19682.

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Photoactivatable β-Lapachones for Targeted Cancer Therapy

Andrew A. Beharry[a], Ivonne R. Lopez-Miranda[a]

[a]*Department of Chemical and Physical Sciences, University of Toronto Mississauga, 3359 Mississauga Road North, Mississauga, L5L1C6, Canada*

Glioblastoma (GBM) is the most common and aggressive primary brain tumor diagnosed in adults. The standard of care is surgical resection followed by radiation and chemotherapy with the alkylating agent, temozolomide (TMZ). Unfortunately, at least one-third of patients experience tumor progression during TMZ adjuvant therapy, due to the presence of intrinsically TMZ-resistant tumor cells. Thus, there is a need for novel therapies to improve current GBM treatments.

ß-lapachone is a small-molecule natural product with potent anti-cancer activity. Its anticancer activity is dependent on the intratumoral activity of the enzyme, NAD(P)H quinone oxidoreductase 1 (NQO1), which mediates a two-electron reduction of ß-lapachone to a hydroquinone that spontaneously oxidizes back to the parent structure, completing a futile redox cycle that, in the process, produces cytotoxic reactive oxygen species (ROS) that kill cancer cells. As GBM has higher NQO1 expression than surrounding brain tissues, ß-lapachone is toxic to cancer cells, whereas normal tissues are unaffected.

Despite its therapeutic promise, the clinical evaluation of ß-lapachone has been limited by its poor water solubility, short in vivo half-life due to rapid metabolism ($t_{1/2}$ = 20 min), and narrow therapeutic window, due to the generation of methemoglobinemia (i.e., oxidized hemoglobin which cannot deliver oxygen to tissues) as a side effect.

To mitigate these limitations, we developed a prodrug of ß-lapachone dependent on light activation [1]. In contrast with native ß-lapachone, our photoactivatable ß-lapachone remained intact in a human whole blood assay ($t_{1/2}$ > 2 h), did not induce methemoglobinemia in mice, and displayed light-induced tumor shrinkage in dorsal window chambered (subcutaneous) pancreatic tumor mice models. The in vitro and in vivo performance of our photoactivatable ß-lapachone will be discussed, along with recent work targeting GBM.

REFERENCES

1. *J. Am. Chem. Soc.,* 2023, **145**(23): 12518-12531

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The Structure and Mechanism of Natural and Engineered Heme Oxygenase Biocatalyts

Stephen G. Bell[a], Matthew N. Podgorski,[a] Joel, H.-Z. Lee[a], Eva F. Hayball,[a] Alecia R. Gee,[a] Tuhin Das[a,] Oghenesivwe Osiebe,[a] Maya L. Doyle & Gashaw Dagnaw,[a]

[a] *University of Adelaide, Adelaide, SA, 5005, Australia*

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Cytochrome P450 heme containing metalloenzymes (CYPs) are monooxygenases which catalyse a diverse range of oxidation reactions through the activation of dioxygen. However, the high cost of the required nicotinamide cofactors and their need for additional electron transfer proteins limits their use as biocatalysts in larger-scale chemical applications. We have recently identified that a family of these CYP enzymes involved in the oxidation of lignin derived aromatics can function as peroxygenases. We have investigated whether other bacterial CYPs can be converted into efficient hydrogen peroxide using peroxygenases through protein engineering of the enzyme's oxygen activation machinery to more closely resemble those of the natural peroxygenase [1,2]. We have developed mutants which have significantly higher peroxygenase activity than a single mutant prototype and that function at significantly lower hydrogen peroxide concentrations [3]. The X-ray crystal structures and other spectroscopic techniques revealed significant structural changes at the heme and the oxygen-binding groove providing a rationale for the modified activity. *In crystall*o reactions and ambient temperature crystallography methods have been undertaken by to shed insight into the mechanism of action of these enzymes [4]. We have extended our mutagenesis strategy to CYP enzymes from a diverse range of bacteria and generated new peroxygenase biocatalysts for the regio- and stereo-selective hydroxylation of steroids, norisoprenoids and drug molecules at relatively low hydrogen peroxide concentrations [5-7]. When this method is applied to CYP enzymes from thermophilic bacteria these reactions can occur at elevated temperatures enabling enzymatic hydroxylation reactions on a variety of substrates under non-standard biological conditions [7].

REFERENCES

1. Podgorski, M. N.; Harbort, J. S.; Lee, J. H. Z.; Nguyen, G. T. H.; Bruning, J. B.; Donald, W. A.; Bernhardt, P. V.; Harmer, J. R.; Bell, S. G. *ACS Catal.* **2022**, *12* (3), 1614-1625.
2. [a] Harlington, A. C.; Shearwin, K. E.; Bell, S. G.; Whelan, F. *Chem. Commun.* **2022**, *58*, 13321–13324. [b] Harlington, A. C.; Das. T. ; :Shearwin, K. E.; Bell, S. G.; Whelan, F. *Nat. Commun.* **2025**, *16*, 1815.
3. [a] Podgorski, M. N.; Akter, J. ; Churchman, L.R.; Bruning, J. B.; De Voss, J.J.; Bell, S. G. *ACS Catal.***2024** *14* (10), 7426-7443 [b] Podgorski, M. N.; Bell, S. G. *ACS Catal.* **2025** *15* (6), 5191–5210
4. Lee, J. H. Z.; Bruning, J. B.; Bell, S. G. *Chem. Eur. J.* **2024**, *30*, e202303335.
5. Lee, J.; Podgorski, M.; Moir, M.; Gee, A. R.; Bell, S. G. *Chem. Eur. J.* **2022**, *28*, e202201366.
6. Akter, J.; Hayball, E. F.; Bell, S. G. *Catal. Sci. Technol.* **2023**, *13*, 6355-6359.
7. [a] Gee, A. R.; Stone, I. S. J.; Stockdale, T. P.; Pukala, T. L.; De Voss, J. J.; Bell, S. G. *Chem. Commun.* **2023**, *59*, 13486–13489. [b] Das. T ; Harlington, A. C.; Hayball E. F.; Bell, S. G. *ChemBioChem*, **2025**, *26* (2) e202400737

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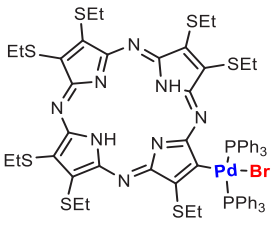
Thioalkyl Porphyrazines: from Materials to Catalysis and Sensing

Sandra Belviso[a], Giuseppe Larotonda[a], Francesco Pizzoli[b], Gabriele Magna[b], Roberto Paolesse[b]

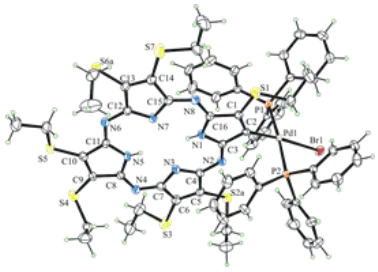
[a] *Dipartimento di Scienze di Base e Applicate - Università della Basilicata, Via dell'Ateneo Lucano 10, I-85100, Potenza, ITALY*
[b] *Dipartimento di Scienze e Tecnologie Chimiche - Università di Roma "Tor Vergata", Via Della Ricerca Scientifica 1, I-00133, Roma, ITALY*

ORALS

Thioalkyl porphyrazines are tetrapyrrolic macrocycles bearing sulfur atoms at the β positions of the ring and exhibiting distinctive optical and electronic properties. Moreover, the presence of sulfur atoms enabled the development of an original and efficient strategy for the non-symmetrical functionalization of the macrocycle with suitable aryl or aryl ethynyl substituents, leading to fine tuning of its electronic properties. As a result, thioalkyl porphyrazines represent promising building blocks for functional materials in optoelectronic applications, such as organic photovoltaics (OPV), nonlinear optics (NLO), and liquid crystals (LC) as we have previously demonstrated. In particular, we reported the application of pyrene-substituted thioalkyl porphyrazines in NLO and OPV,[1] as well as the preparation of their composites with nanocarbons, yielding materials capable of efficient photocurrent generation.[2] More recently, we also described a new porphyrazine scaffold conjugated with a chiral, extended aromatic hexahelicene moiety, a structural motif that remains largely unexplored in OPV applications.[3] We will describe herein the synthesis of the novel β-η¹-Pd(II)-thioethyl porphyrazine complex **1**, as well as its structural and electronic properties, and potential application in material science and as a catalyst in cross-coupling reactions.[4] Moreover, considering that tetrapyrrolic systems have been extensively exploited as sensing materials in chemical sensors,[5] we explored, for the first time, the potential of thioalkyl porphyrazines in this field. A selected set of these compounds was employed as sensing layers on quartz crystal microbalance (QCM) transducers to discriminate a series of amines, alcohols, and alkanes using an electronic-nose approach. The influence of the thioalkyl chain length and of different metal coordination within the macrocyclic cavity on sensing performance was systematically evaluated.



(1)



REFERENCES

1. Belviso, S.; Tessore, F.; Santoro, E.; Righetto, S.; Penconi, M. *J. Phys. Chem. C* **2019**, *123*, 13074.
2. Belviso, S.; Capasso, S.; Santoro, E.; Najafi, L; Lelj, F.; Superchi, S.; Casarini, D.; Villani, C.; Spirito, D.; Bellani, S.; Del Rio Castillo, A. E.; Bonaccorso, F. *Adv. Funct. Mater.* **2018**, 1705418.
3. Belviso, S.; Marsico, G.; Franzini, R.; Villani, C.; Abbate, S.; Longhi, G. *Dalton Trans*. **2022**, *51*, 16453.
4. Belviso, S.; Larotonda, G.; Santarsiere, A.; Santoro, E. ; Tuzi, A. *Dalton Trans*. **2025**, *541*, 11563.
5. Paolesse, R.; Nardis, S.; Monti, D.; Stefanelli, M.; Di Natale, C. *Chem. Rev*. **2017**, *117*, 2517.

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Progression on the Development of Boron Subphthalocyanines, Subnaphthalocyanines and Hybrids for their Applications and on the Sustainability Side.

Timothy P. Bender[a,b,c,d], Jennifer Tong[a], Andrew Jo[a] and Keerthikah Jegatheesan[a]

[a] *Department of Chemical Engineering and Applied Chemistry. University of Toronto. 200 College Street, Toronto, Ontario, CANADA*
[b] *Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario, CANADA M5S 3H6*
[c] *Department of Materials Science and Engineering, University of Toronto, 184 College Street, Toronto, Ontario, CANADA M5S 3E4*
[d] *Department of Mechanical and Industrial Engineering, University of Toronto, 5 King's College Road, Toronto, Ontario, Canada M5S 3G8*

For many years, my group has been focused on the molecular/material designs, synthesis and applications of boron subphthalocyanines (BsubPcs) and subnaphthalocyanines (BsubNcs), which are macrocycles with a chelated central boron atom.[1] Our focal points continues to be between the basic and applied chemistry and their application into organic photovoltaics (OPVs)/organic solar cells (OSCs),[2a] batteries, and organic light emitting diodes (OLEDs);[2b] electrochemical and photophysical properties being critical to these applications. [2c-d] To-date/in the literature and industry, there is always significant energy that needs to go into Pc formation/ manufacture and therefore we are also considering a more sustainable process to make the Pcs as well as the BsubPc and BsubNcs.

For this presentation, a point will be our progress on the development of BsubNcs. In the past we have shown that BsubNcs end up being a mixed alloyed composition based on bay-position halogenation that was formed randomly during the reaction of BCl_3 with 2,3-dicyanonaphthalene, however the random halogenation has been shown to have a positive impact to the OPV devices,[3a] but negative within OLED devices.[3b] We did develop a method to separate the mixed alloyed BsubNcs, and it was a mixed set of bands and we acquire data to show the impact of the percentage/number of bay-position halogens, including chlorine and bromine, on electrochemical/conductivity etc.[4a-b] I will also present a new synthetic methodology to avoid the random bay-position halogenation of the BsubNcs. And I will also present a new method to have complete bay-position halogenation to the BsubNcs, is ongoing research to-date. We have also applied a computational model to look at the relative impact of the random bay-position halogenation on the electronics, the HOMO-LUMO levels as well, so I will likely present that as well. I may likely also present that we ongoing considerations of other bay-position substitutions of the BsubNcs to avoid the random halogenation. Re hybrids, have recently developed BsubNc + BsubPc hybrid materials and to-date of filing the abstract we have setup another method and we are likely to achieve this by this summer, then I will present its outcome. I will also likely outline our approach to accelerate the development of BsubNcs + BsubPcs + hybrids whereby their molecular design can be first justified through a computational model. Next, I will present recent outcomes that enables the BsubPc and BsubNc formation via having lower embodied energy and therefore can have more sustainability for any upcoming studies, their application, etc, and can also apply to phthalocyanines (Pcs).

REFERENCES

1. Lavarda, G.; *et al*, Chem. Soc. Rev., **2022**, *51*, 9482-9619.
2. First examples, many more available in literature over time: (a) Morse, G. E.; Bender, T. P., *ACS Appl. Mater. Interfaces* **2012**, *4* (10), 5055-5068. (b) Plint, T. G.; *et al.*, *Opt. Mater.* **2018**, *75*, 710-718. (c) Grant, T. M.; *et al*., *Chem. Rec.* **2019**, *19* (6), 1093-1112. (d) Sampson, K. L.; *et al*. *J. Phys. Chem. A* **2018**, *122* (18), 4414-4424.
3. (a) Dang, J. D.; *et al*. *J. Mat. Chem. A* **2016**, *4* (24), 9566-9577. (b) Jones, S.T.E.; *et al.*; *ChemRxiv*. **2020**, https://doi.org/10.26434/chemrxiv.13366190.v1.
4. (a) Holst, D.; *et al.*; *New J. Chem.*, **2021**, 45, 5791. (b) Holst, D.; *et al.*; *New J. Chem.*, **2021**, 45, 21082.

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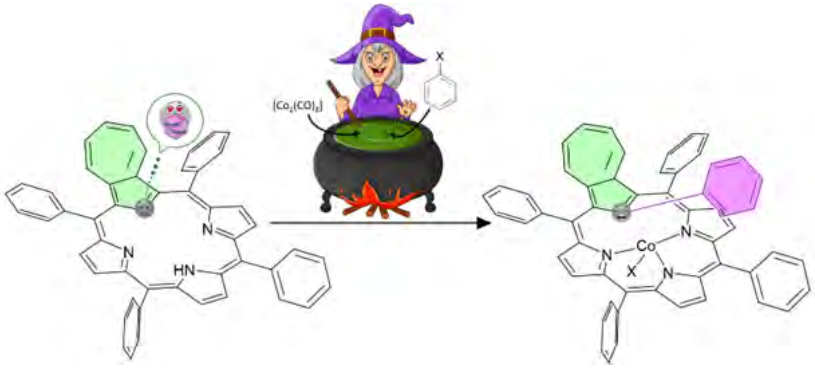
Regioselective arylation and coordination cavity magic in carbaporpyrinoids

Michał J. Białek[a], **Wiktoria Bara**[a], **Kinga Szydełko**[a]

[a]*Department of Chemistry, Univeristy of Wrocław, F. Joliot-Curie 14, 50383 Wrocław, Poland, michal.bialek@uwr.edu.pl*

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Functionalization of the carbaporphyrin core influences its framework and spectroscopic properties, as the planarity is no longer possible. There is no more room for regular coordination, as there is an additional steric hindrance [1]. Yet, forced proximity of the substituent may result in new chemistry induced by a metal-ion insertion and occurring in the coordination core as well as at the porphyrinoid periphery [2,3].
Here, we present cobalt-induced inner carbon arylation in a series of carbaporphyrinoids [4,5]. The reaction results in a paramagnetic complex (and a diamagnetic one for N-confused porphyrin) that undergoes facile demetallation to give the respective functionalized ligand.
The phenyl substituent confined in the coordination core, while anchored to the inner carbon atom, alters the coordination properties. It also induces a series of transformations within the macrocycles when exposed to palladium(II) or rhodium(III) ions. Especially susceptible is azuliporphyrin, which gets oxidized, reduced or contracted to accommodate the incoming metal ion. Structures are characterized with HRMS, NMR and SC-XRD.



REFERENCES

1. M.J. Białek, K. Hurej, H. Furuta, L. Latos-Grażyński, Organometallic chemistry confined within a porphyrin-like framework, *Chem. Soc. Rev.* 2023, 52, 2082
2. K. Hurej, M. Pawlicki, L. Szterenberg, L. Latos-Grażyński, A Rhodium-Mediated Contraction of Benzene to Cyclopentadiene: Transformations of Rhodium(III) m-Benziporphyrin. *Angew. Chem. Int. Ed.* **2016**, 55, 1427
3. K. Szymanowski, W. Bara, M.J. Białek, Cobalt-Assisted α-Activation of Ketones, Their Arylation and Keto-Enol Equilibrium Confined into a Macrocycle. *Chem. Eur. J.*, **2025**, 31, e202500906
4. For similar reactivity see: B.J. Foley, C.M. Palit, S.D. Timpa, O.V. Ozerov, Synthesis of (POCOP) Co(Ph)(X) pincer complexes and observation of aryl–aryl reductive elimination involving the pincer aryl. *Organometallics* **2018**, 37, 21, 3803
5. C.R. Liu, Y.Y. Qian, K.S. Chan, Base-promoted aryl–bromine bond cleavage with cobalt(II) porphyrins via a halogen atom transfer mechanism. *Dalton Transactions* **2014**, 43, 21, 7771

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Sensing and Imaging with Red to NIR Emitting Metalloporphyrin and Aza-BODIPY Dyes

Sergey M. Borisov,[a] Ruslan I. Dmitriev,[b] Angela C. Debruyne,[b] Irina A. Okkelman,[b] Giulia Ceriotti,[c] Georg Schwendt,[a,d] Andreas Matijevic,[a] Torsten Mayr[a], Michael Kühl[d]

[a] *Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Graz, Austria*
[b] *Department of Human Structure and Repair, Ghent University, Ghent, Belgium*
[c] *Institute of Earth Surface Dynamics, University of Lausanne, Lausanne, Switzerland*
[d] *Department of Biology, University of Copenhagen, Helsingor, Denmark*

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Recent progress in sensing and imaging with functional dyes based on (metallo)porphyrins and aza-BODIPYs will be highlighted. Simultaneous imaging of oxygen and temperature is realized with quinone-extended porphyrin complexes [1, 2]. These dyes feature dual emission (phosphorescence and thermally-activated delayed fluorescence) which ratio is temperature-dependent whereas the luminescence decay time is affected primary by oxygen concentration. This rare behavior enables dual sensing and imaging by measuring the luminescence decay time and luminescence ratio.

Capitalizing on the spectral properties of the benzoporphyrin complexes (absorption in the red and emission in the NIR part of the spectrum) we demonstrate their utility for oxygen imaging in a wide range of biological probes. Dye-doped nanoparticles are utilized for *in vivo* imaging of oxygen dynamics in corals utilizing decay-time based read-out [3]. In order to enable broader adoption of such materials we introduce a new imaging set-up based on a compact and affordable gate-able CMOS camera that utilizes multiple exposure in one frame capability [4]. For microscopy applications we present a ratiometric 2-wavelength system based on combination of a NIR-emitting Pt(II) benzoporphyrin and a red-emitting aza-BODIPY dye simultaneously excited with red light. The nanoparticle-based system is utilized for imaging of oxygen distribution in multicellular spheroids revealing inverse oxygen gradients [5] whereas a planar foil is shown to be excellently suited for simultaneous real-time imaging of oxygen gradients and microbial community special organization in confined environments. The community consists of two bacterial strains representing distinct phenotypes—elongated and rounded cell shapes—engineered to express mScarlet-I and GFP, respectively, which can be imaged simultaneously with red-NIR emitting O_2 sensors.

A new fluorescent aza-BODIPY dye modified with an aniline-based receptor shows “off-on” response to pH in the acidic range due to inhibition of photoinduced electron transfer upon protonation of the receptor. Immobilization of this indicator into a hydrogel matrix protected by a silicone membrane gives a highly sensitive and robust ammonia sensor which proved suitable for monitoring this analyte, that is highly toxic for fish, in natural waters.

Finally, we demonstrate utility of an aza-BODIPY dye as a NIR emitter for visualizing the internalization and biological impact of nanoplastics in live intestinal organoids by Fluorescence Lifetime Imaging Microscopy [6].

REFERENCES

1. Schwendt, G.; Borisov, S. M. *Sens. Actuators B: Chem.* **2023**, *393*, 134236
2. Schwendt, G.; Kalinichev, A. V.; Borisov, S. M.; Koren, K. *ACS Meas. Sci. Au* **2024**, *4*, 568–576
3. Kühl, M.; Nielsen, D. A.; Borisov, S. M. *ACS Sens.* **2024**, *9*, 4671–4679
4. Rousseau, G. et al. *Sens. Actuators B: Chem.* **2026**, *447*, 138849
5. Debruyne, A. C. et al. *ACS Nano* **2024**, 18, 12168–12186
6. Okkelman, I. A. et al. *Light Sci Appl* **2025**, 14, 272

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Fused MetalloPorphyrins Thin Films for the Heterogeneous Electrocatalytic Conversion of Small and Low Energy Molecules into Advanced Chemicals

Nicolas D. Boscher[a]

[a] *Luxembourg Institute of Science and Technology, 28 Avenue des Hauts-Fourneaux, Esch-sur-Alzette, L-4362 Luxembourg*

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Metalloporphyrins are distinguished by their extended π-conjugated macrocycles and redox-active metal centers, which can reversibly access multiple oxidation states and play central roles in biological energy conversion processes such as photosynthesis and respiration. Beyond their molecular properties, several studies have demonstrated that covalent conjugation between metalloporphyrin units induces cooperative effects that markedly enhance catalytic performance. In particular, superior catalytic activities have been correlated with the ability of conjugated porphyrin assemblies to accumulate and delocalize multiple charges, thereby enabling demanding multi-electron reaction pathways. Within this context, fused porphyrin tapes—linear arrays of porphyrin units covalently fused through their meso and β positions—represent an appealing architecture, as they form rigid, highly π-conjugated, and electrically conductive systems [1]. Nevertheless, despite the vast structural diversity accessible within porphyrin chemistry, the application of fused porphyrin tapes remained largely unexplored.

Oxidative chemical vapor deposition (oCVD) has recently emerged as an effective strategy for the direct fabrication of fused porphyrin tapes as thin films [2]. In this vapor-phase process, oxidative dehydrogenative C–C coupling and in situ doping occur concurrently upon co-delivery of the monomer and oxidant to the substrate surface [3]. Using this approach, metalloporphyrins featuring unsubstituted meso positions can be successfully converted into extended fused porphyrin tapes. A key advantage of oCVD lies in its ability to deposit uniform, thickness-controlled films on a wide range of substrates, making it particularly attractive for electrocatalytic applications. Notably, the polymerization process is largely insensitive to the nature of peripheral substituents [4] or the identity of the central metal ion [5], offering substantial flexibility for tuning electrocatalytic functionality.

In this study, we demonstrate the potential of fused porphyrin tape thin films as highly active electrocatalysts for the hydrogen evolution reaction (HER) [6], nitrate reduction reaction (NO_3RR), oxygen reduction reaction (ORR), and oxygen evolution reaction (OER) [7]. Combined experimental and computational studies reveal that both the metal center and the porphyrin substitution pattern significantly influence catalytic performance. Overall, this work establishes a versatile platform for the rational design and seamless integration of metalloporphyrin-derived electrocatalysts into advanced energy conversion systems.

REFERENCES

1. T. Tanakaa, A. Osuka, *Chemical Sociaty Review*, **2015**,*44*, 943-969.
2. G. Bengasi, K. Baba, G. Frache, J. Desport, P. Gratia, K. Heinze, N. D. Boscher, *Angew. Chem.*, **2019**, *131*, 2125-2130
3. M. Heydari Gharahcheshmeh, K. K. Gleason, *Adv. Mater. Interfaces*, **2019**, *6*, 1801564
4. D. Bansal, S. Ganesh Moorthy, M. Bouvet, N. D. Boscher, *ACS Appl. Mater. Interfaces*, **2024**, *16*, 68091-68102
5. D. Cardenas-Morcoso, E. Vey, M. Heiderscheid, G. Frache, ,N. D. Boscher, *J. Mater. Chem. C*, **2022**, *10*, 2194-2204
6. A. M. Huerta-Flores, G. Bengasi, K. Baba, N. D. Boscher, *ACS Appl. Energy Mater.*, **2020**, *3*, 9848-9855
7. D. Bansal, D. Cardenas-Morcoso, N. D. Boscher, *J. Mater. Chem. A*, **2023**, *11*, 5188-5198

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Porphycene Thin Films as Optically Reversible Chemosensors in 2D and 3D Architectures

Alberto Bossi[a], M. Penconi[a], J. Waluk[b], A. Listkowski[b], A. Gajewska[b], A. Antonello[a], G. Bussetti[d]

[a] *Istituto di Scienze e Tecnologie Chimiche "Giulio Natta" del Consiglio Nazionale delle Ricerche, CNR-SCITEC, v. Fantoli 16/15, I-20138 Milano (Italy); SmartMatLab Center, v. Golgi 19, II-20133 Milano (IT)*
[b] *Institute of Physical Chemistry, Polish Academy of Science, 01-224 Warsaw, Kasprzaka 44/52 (PL); Faculty of Mathematics and Science, Cardinal Stefan Wyszyński University, Dewajtis 5,01-815 Warsaw (PL)*
[d] *Department of Physics, Politecnico di Milano, p.za Leonardo da Vinci 32, I-20133 Milano (IT)*

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Molecular materials with tailored optical properties represent valuable platforms for advanced sensing applications. In particular, chemoresponsive systems are essential for the selective and sensitive detection of small analytes, with important implications for environmental monitoring, medical diagnostics, and industrial quality control. A key challenge in this field is the development of reversible signaling mechanisms—especially optical ones—that enable continuous and real-time detection. Porphycenes (H2Po), tetrapyrrole macrocycles constitutional isomers of porphyrins,[1] are chemically and thermally stable 18π electron conjugated chromophores that can serve as versatile scaffolds due to their rich peripheral functionalization possibilities (R^1 and R^2 in Fig. 1), which can be engineered for specific applications. In this study, three porphycenes (Fig. 1) were investigated: the parent compound **1**, and two tetra-alkyl-substituted derivatives bearing four n-propyl groups either at the *β* positions of the pyrrole rings (**2**) or at the *meso* positions (**3**). *β*-alkyl substitution (**2**) should not significantly impact the electronic densities of the molecular core, whereas *meso* functionalization (**3**) tend to distorts the core from almost planar towards more strongly rectangular structure compared to that present in **1** and **2**. The acidochromic behaviour of the three porphycenes was investigated both in solution and in the solid state, [2] including three-dimensional neat films and polymer-dispersed matrices. Optical absorption and photoluminescence measurements reveal distinct spectral signatures associated with the protonated and unprotonated forms of the porphycenes, as well as differences in their stability and reversibility, highlighting the potential of porphycene-based thin films as optically reversible chemosensing platforms.

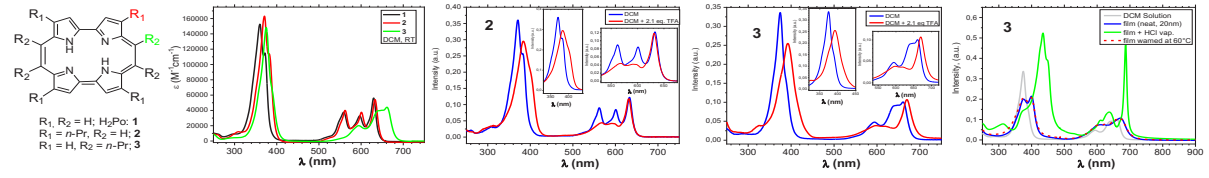


Figure 1: a) chemical structures of the studied porphycenes; b) compararisons of the optical absorptivities of **1**,**2**,**3** in DCM solutions; c, d) changes in optical absorptions of **2** and **3** upon addition of 2 equiv. of H^+; e) changes in optcal absorptions of a 20nm thin film of **3** when exposed to HCl vapours.

1. E. Vogel, M. Köcher, H. Schmickler, J. Lex, *Angew. Chem. Int. Ed. Engl*. **1986**, 25, 257.
2. A. Bossi, J. Waluk, R. Yivlialin, M. Penconi, M. Campione, G. Bussetti, *ChemPhotoChem,* **2020**, 4, 5264

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Tailoring Electronic Properties in π-Extended Porphyrin-based Nanostructures through Bottom-Up Fabrication

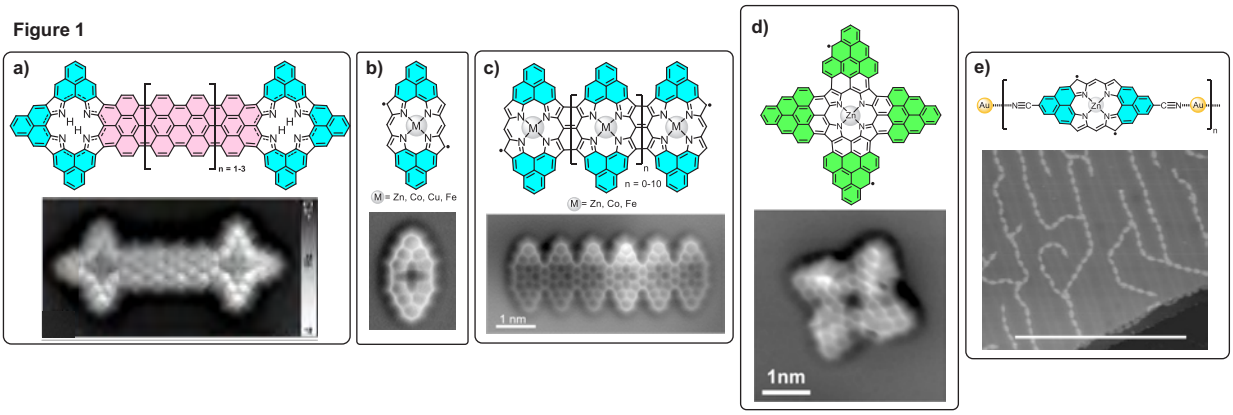
Giovanni Bottari,[a,b,c] Miguel Martínez García,[a,b] Sergio Ligos,[a,b] Tomás Torres,[a,b,c] Feifei Xiang,[d] Roman Fasel,[d] and David Écija[c]

[a] *Departamento de Química Orgánica, Universidad Autónoma de Madrid, 28049 Madrid, Spain*
[b] *IMDEA-Nanociencia, Campus de Cantoblanco, 28049 Madrid, Spain*
[c] *Institute for Advanced Research in Chemical Sciences (IAdChem), 28049 Madrid, Spain*
[d] *Empa-Swiss Federal Laboratories for Materials Science, 8600 Dübendorf, Switzerland*

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Since its inception nearly two decades ago, on-surface synthesis (OSS) has matured into a powerful technique for constructing π-extended nanostructures on surfaces—structures that are often unattainable through conventional solution-phase routes.[1] Among the building blocks used for the fabrication of such nanoarchitectures, porphyrins (Pors) are of particular interest due to their planar structure with an aromatic core of 18 π-electrons, remarkable thermal stability, tunable redox properties, and intense optical features.[2] Herein, we present our endeavor towards the on-surface fabrication, and structural and electronic characterization of Por-based systems such as Por-graphene nanoribbon hybrids (Figure 1a),[3a,c] phenalenyl (Figure 1b)[3b,e] and [3]triangulene-fused (Figure 1d)[3h,i] π-extended Por monomers, Por nanotapes (NTs) (Figure 1c),[3d,g] and Por-based metalo-organic 1D nanochains (Figure 1e),[3f] many of such structures showing an open-shell character.

Figure 1



REFERENCES

1. S. Clair, D. G. de Oteyza, *Chem. Rev.* **2019**, *119*, 4717-4776.
2. K. M. Kadish, K. M. Smith, R. Guilard, The Porphyrin Handbook, Vol. 1-10, Academic Press, Burlington, 2000.
3. a) L. M. Mateo et al., *Angew. Chem. Int. Ed.* **2020**, *59*, 1334-1339; b) Q. Sun et al., *J. Am. Chem. Soc.* **2020**, *142*, 18109-18117; c) L. M. Mateo et al. *Chem. Sci.* **2021**, *12*, 247-252; d) Q. Sun et al. *Angew. Chem. Int. Ed.* **2021**, *60*, 16208-16214; e) Q. Sun et al. *Adv. Sci.* **2022**, *9*, 2105906 (1-9); f) M. Tenorio et al. *Angew. Chem. Int. Ed.* **2025**, *64*, e202420572(1-9); g) R. Robles et al., *Angew. Chem. Int. Ed.* **2025**, *64*, e15342(1-7); h) M. Martínez García et al., *Submitted manuscript*; i) *Work in progress*.

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Ambipolar porphyrinoid-based gas sensors: Inversion of polarity through external stimuli

Marcel Bouvet[a]

[a]*Institut de Chimie Moléculaire de l'Université de Bourgogne, CNRS UMR 6302, Université Bourgogne Europe, 9 avenue Alain Savary, BP47870 Dijon cedex, France ; marcel.bouvet@ube.fr*

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In the present work, we successfully synthesised a series of phthalocyanine complexes with varying the number and nature of halogen (F_0, F_8, F_{16} and Cl_8) and metal centre (Co, VO, Zn and Cu). We fabricated bilayer heterojunction sensors with $LuPc_2$ as a common top layer on these molecules as sublayers, and investigated their sensing properties towards both oxidizing and reducing gaseous species (NH_3, NO_2 and O_3). The resulting heterojunction devices exhibit p-type, n-type or ambipolar (both p- and n-type) behaviours, depending on an external trigger (Fig. 1a). We will see, from examples, that light, temperature, humidity and applied potential can be able to switch the polarity of majority charge carriers, leading to a positive or negative response to a given gas (Fig. 1b).

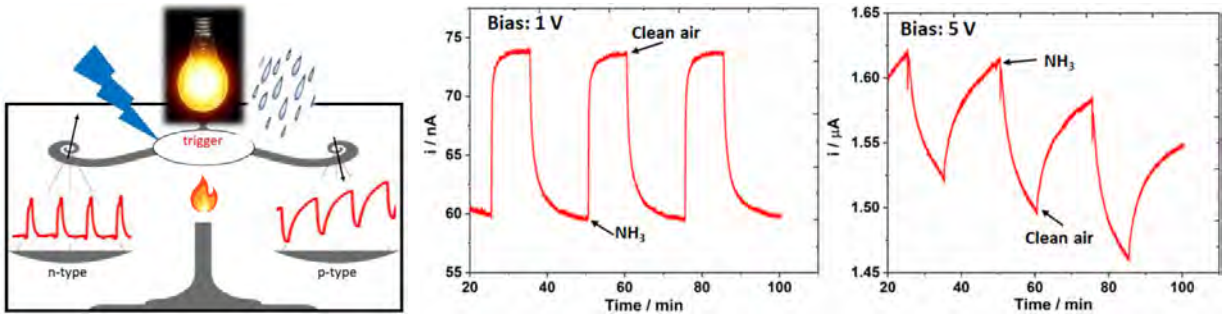


Fig. 1: a) *Schematic view of triggers (voltage, light, humidity and temperature) capable of changing polarity from n-type to p-type and b) current variation of a heterojunction towards NH_3 under successive exposure/recovery cycles.*

REFERENCES

1. A. Kumar, C. H. Devillers, R. Meunier-Prest, D. Sabat, E. Lesniewska, M. Bouvet, Bias induced ambipolar transport in organic heterojunction sensors, *Adv. Electron. Mater*., 2400865, **2025**.

2. S. Ganesh Moorthy, A. Apoubou, S. Ouedraogo, L. Vachey, M. Bayo-Bangoura, M. Bouvet, In-depth study of ambipolar charge transport regime through external triggers and gas sensing, *ACS Appl. Mater. Interfaces,* 16, 58991-59003, **2024**.

3. S. Ganesh Moorthy, S. Ouedraogo, M. Bouvet, Ambipolar heterojunction sensors: Another way to detect polluting gases, *ACS Sensors*, 9, 3707-3719, **2024**.

4. S. Ganesh Moorthy, M. Bouvet, Effects of visible light on gas sensors: From inorganic resistors to molecular material-based heterojunctions, *Sensors*, 24, 1571, **2024**.

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Cobalt Cytochrome Catalysts for CO_2 Conversion

Kara L. Bren[a], Karishma B. Ramesh[a], Alison A. Salamatian[a], María Fernanda Lizarazo[a], Linda Leone[b], Angela Lombardi[b]

[a]*Department of Chemistry, University of Rochester, Rochester, NY 14627-0216 USA*
[b]*Department of Chemical Sciences, University of Naples Federico II, 80126, Naples, Italy*

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Developing CO_2 as a building block to produce a range of products is of high current interest. A primary challenge in the activation and conversion of CO_2 to useful products is suppressing the competing hydrogen evolution reaction. For catalysts functioning in water, a desired solvent and proton source, selectively reducing CO_2 is particularly challenging. Developing this chemistry in a photochemical system presents additional barriers to achieving selectivity because reactions of photosensitizers also impact system product distribution.

Here, we report the use of a cobalt-substituted cytochrome *c* fragment (CoMP11-Ac) as well as a synthetic cytochrome *c* mimic (CoMC6*a, "mimochrome") for the electrochemical and photochemical reduction of CO_2 to CO, achieving selectivity for CO production exceeding 90% in optimized electrochemical conditions, and exceeding 50% in photochemical conditions. In electrocatalytic systems, we demonstrate that selectivity depends on applied potential and the pK_a of the proton source (in water, protonated buffer species). We propose that avoiding formation of a formal Co(I) species by avoiding highly cathodic potentials and the use of relatively basic proton donors favors CO over H_2 production [1,2]. Furthermore, we find that the relatively enclosed active site of CoMC6*a relative the solvent-exposed active site of CoMP11-Ac impacts proton delivery kinetics and reaction selectivity. These concepts have also been shown to apply to photochemical systems for CO_2 reduction, with the proton donor acidity, photosensitizer reduction potential and catalyst Co(II/I) potentials dictating system activity and selectivity. This study demonstrates the complex interplay between proton donor pK_a, the potential of electrons supplied to the catalyst, and the catalyst active-site structure in determining CO_2 reduction activity and selectivity for these structurally related biocatalysts.

REFERENCES

1. Potential- and Buffer-Dependent Selectivity for the Conversion of CO_2 to CO by a Cobalt Porphyrin-Peptide Electrocatalyst in Water, Jose L. Alvarez-Hernandez,‡ Alison A. Salamatian,‡ Ji Won Han, and Kara L. Bren,(‡contributed equally), ACS Catal., 2022, 12, 14689-14697. DOI: 10.1021/acscatal.2c03297
2. Electrocatalytic CO_2 Reduction by a Synthetic Cobalt Porphyrin Mini-Enzyme. Alison A. Salamatian, Jose L. Alvarez-Hernandez, Karishma B. Ramesh, Linda Leone, Angela Lombardi, Kara L. Bren, Chem. Sci., 2025, 16, 5707-5716. Spotlight Collection on Bioinorganic Chemistry. DOI: 10.1039/D4SC07026G

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Main Group Corroles

Martin Bröring[a]

[a]*IAAC, TU Braunschweig, Germany*

The vast majority of metal corroles are complexes of transition metals. For those, the redox behaviour and chemical reactivity of the axial ligands play a decisive role, and typical topics include the stabilisation of particularly high oxidation states and the non-innocent behaviour of the corrole ligand.

In contrast, the numerically significantly inferior main-group corroles mostly represent electronically innocent, diamagnetic species without unpaired electrons. In this field, topics from photochemistry and photophysics are therefore particularly relevant, and structural properties are more important than electronic characteristics.

In this lecture, our investigations into the syntheses, chemical behaviour and photophysical investigations of main group corroles[1,2] will be presented, using various current examples.

REFERENCES

1. V. Caliskanyürek, S. Eulberg, O. Lange, M. Bröring, S. Tschierlei, *Chem. Commun.* **2024**, *60*, 4096-4099.
2. S. Eulberg, N. Schulze, J. Krumsieck, N. Klein, M. Bröring, *Angew. Chem.* **2023**, *132*, e202306598; *Angew. Chem. Int. Ed.* **2023**, *62*, e202306598.

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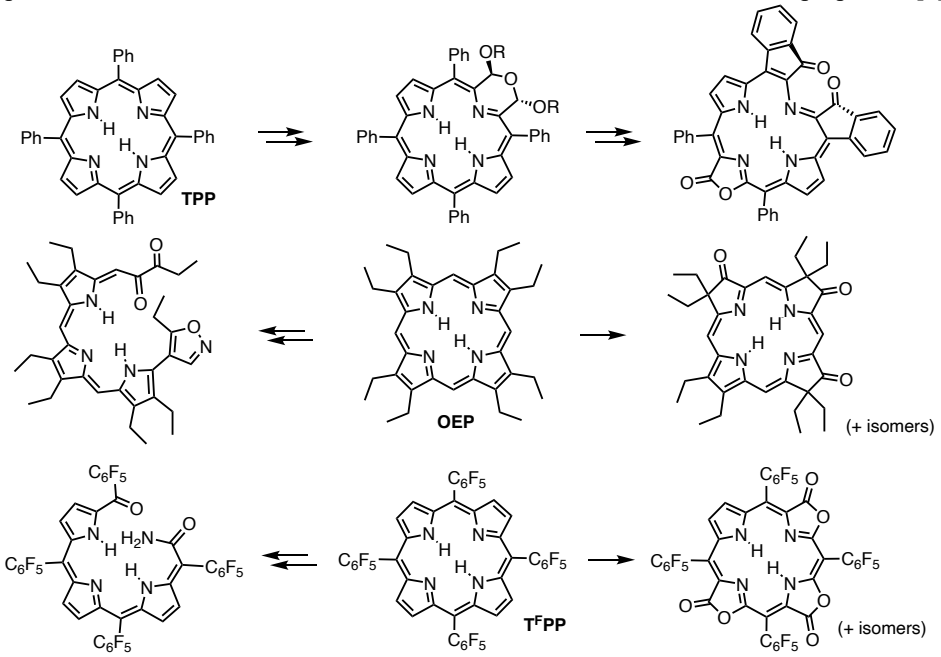
Converting porphyrins into exotic porphyrinoids

Christian Brückner

Department of Chemistry, University of Connecticut, Storrs, CT 06269-3060, USA.

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The step-wise conversion of one, two, or three pyrrolic building blocks in well-known porphyrins, such as *meso*-tetraaryl- (**TPP** and **T^{F}PP)** and ß-octaalkyl-porphyrins (**OEP)**, to non-pyrrolic building blocks has shown to be a versatile approach toward the formation of exotic porphyrinoids. While some still possessed porphyrin-like electronic properties and structures, some showed much altered electronic and chemical properties [1].



We will provide an overview of some well-known and unpublished systems with focus on what electronic or chemical properties distinguishes them as exotic [2]. Examples of exotic physical properties include unusually shifted optical spectra and modulations of their aromaticity [3]. We will present recent data on the identification of the pyrrole-modified porphyrinoid fragments found under ESI+ mass spectrometry conditions [4]. Exotic chemical properties include their intervonversions or chirality imposed onto them by means of their unusual conformations [5] and their ring-opening reactions involving the cleavage of a pyrrolic building block [6].

REFERENCES

1. Brückner, C. *Acc. Chem. Res.* **2016**, *49*, 1080.
2. Nevonen *et al. J. Phys. Chem. A.* **2024**, *128*, 24, 4823.
3. (a) Chaudhri, N. *et al. Chem. Sci.* **2021**, *12*, 12292. (b) Hewage, N. *et al. J. Org. Chem.* **2022**, 87, 12096. (c) Chaudhri, N. *et al. J. Org. Chem.* **2022**, *87*, 7179.
4. Greis, K. *et al. J. Am. Soc. Mass Spectrom.* **2026**, *37*, 289.
5. Brückner, C. *et al. J. Am. Chem. Soc.* **2011**, *133*, 8740.
6. Hewage, N. *et al. J. Org. Chem.* **2024**, 89, 6584.

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Heme-Dependent CO Sensing Transcription Factors: CooA and RcoM

Judith N Burstyn[a], Madeleine G. Roberts[a], Matthew R. Dent [b], Brian R. Weaver[a], Christopher E. Berndsen[c]

[a]*University of Wisconsin-Madison, Madison, WI, USA*
[b]*Wayne State University, Detroit, MI, USA*
[c]*James Madison University, Harrisonburg, VA, USA*

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Two known heme-dependent transcription factors, CooA and RcoM, regulate inducible carbon monoxide metabolism pathways in anaerobic and aerobic microorganisms, respectively. In these bacteria and archea, CO is a source of energy and carbon, and the enzymes that oxidize CO use complex metallocofactors that depend on accessory proteins for assembly and proper function. The high energetic cost of these processes necessitates that gene expression occurs only when CO concentrations and redox conditions are appropriate.[1]

CooA is a cAMP receptor protein / fumarate and nitrate reductase superfamily protein. Allosteric activation of CooA in response to CO binding has been described in terms of discrete structural changes, without consideration of a potential role for protein dynamics in DNA binding. We used site-directed spin-label electron paramagnetic resonance spectroscopy (SDSL-EPR) to probe slow timescale (μs-ms) conformational dynamics of CooA with the redox-stable MAL-6 nitroxide spin label, and IR spectroscopy to probe the environment at the CO-bound heme. Cysteine substitution variants were created to selectively label CooA in key functional regions, the heme-binding domain, the 4/5-loop, the hinge region, and the DNA binding domain. The EPR spectra of labeled CooA variants were compared across three functional states: Fe(III) “locked off”, Fe(II)-CO “on”, and Fe(II)-CO bound to DNA. We observed changes in the multicomponent EPR spectra, most notably in the hinge region and DNA binding domain, broadening the description of the CooA allosteric mechanism to include protein dynamics in DNA binding. DNA-dependent changes in IR vibrational frequency and band broadening suggest that DNA binding alters the environment of the heme-bound CO.[2]

RcoM is a single-component transcription factor with a PAS-type sensory domain connected via a long, unstructured linker to a LytTR-type DNA binding domain. Absent structural data for RcoM in any functional state, it remains unclear how carbon monoxide binding at heme leads to DNA binding. We report low-resolution solution structural models of the RcoM dimer and of the RcoM:DNA complex, which consists of two RcoM dimers and a 62 bp promoter DNA sequence, made using size-exclusion chromatography coupled small-angle X-ray scattering. A protein structure prediction model, refined with experimental data, shows dimerization occurring through the PAS domains, with non-interacting LytTR domains. We show that RcoM does not change oligomeric state in response to effector-binding; instead, our data implies that two RcoM dimers independently bind the triplet direct repeat promoter sequence. This work offers a first step in the structural characterization of a unique transcription factor, widening our understanding of DNA binding mechanisms among LytTR-proteins.[3]

REFERENCES

1. M. R. Dent, B. R. Weaver, M. G. Roberts, J. N. Burstyn, *J. Bacteriology*, **2023,** *205(5)*, 1-18
2. M. G. Roberts, M. R. Dent, S. Ramos, M. C. Thielges, J. N. Burstyn *J. Inorg. Biochem.* **2024**, *259*, 112656
3. M. R. Dent, M. G. Roberts, H. E. Bowman, B. R. Weaver, D. R. McCaslin, J. N. Burstyn *Biochemistry* **2022**, *61,* 678−688

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Porphyrins in Third-Generation Organic Solar Cells: Architectural Insights and Design Strategies

Rubén Caballero, Lina F. Castaño, Pilar de la Cruz

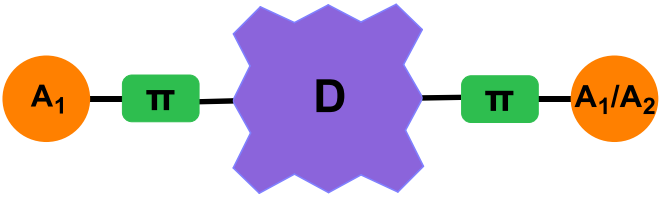
Instituto de Nanociencia Nanotecnología y Materiales Moleculares (INAMOL), Universidad de Castilla-La Mancha, Toledo, Spain.

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Porphyrins, with their exceptional light-harvesting capability and tunable electronic properties, have been used as semiconductors in bulk-heterojunction organic solar cells. Push-pull systems based on porphyrins are designed with architectures such as donor–acceptor (D–A), acceptor–donor–acceptor (A–D–A), and donor–acceptor–donor (D–A–D) configurations. These designs enable broad absorption profiles extending into the near-infrared region and facilitate favourable energy level alignment for efficient exciton dissociation. [1]

Over the last few years, advances from our research group have highlighted the versatility of porphyrins in constructing advanced active phases for OSCs and underscored their potential in achieving high-efficiency, solution-processable photovoltaic devices, delivering power conversion efficiencies (PCEs) exceeding 13% in binary blends[2] and up to 16% in ternary devices.[3] Recently, we have explored the use of non-conventional asymmetric π-conjugated systems incorporating aromatic and non-aromatic scaffolds for their development in organic electronics. [4]

Here we present our latest work, aimed at further advancing the performance of porphyrin-based organic electronics. To gain deeper insight into the effect of molecular symmetry, we have designed novel porphyrin-based semiconductors featuring a unique architecture.



REFERENCES

1. Caballero, R., de la Cruz, P., Sharma, G.D., Langa. F. *Coord. Chem. Rev.* **2026,** *548,* 217199.
2. Caballero, R., Domínguez, R., Shyam Shankar, S., Privado, M., Prieto, P., de la Cruz, P., Singhal, R., Sharma, G.D., Langa, F., *Solar RRL*, **2024,** *8(10),* 2400069.
3. Caballero, R., de la Cruz, P., Langa, F., Singhal, R., Sharma, G. D. *ChemSusChem,* **2025,** e202402495.
4. Privado, M., Moles Quintero, S., de La Cruz, P., Barrejón, M., Babu, J., Casanova, D., Langa, F., Casado, J., *Angew. Chem. Int. Ed.,* **2024**, e202413988.

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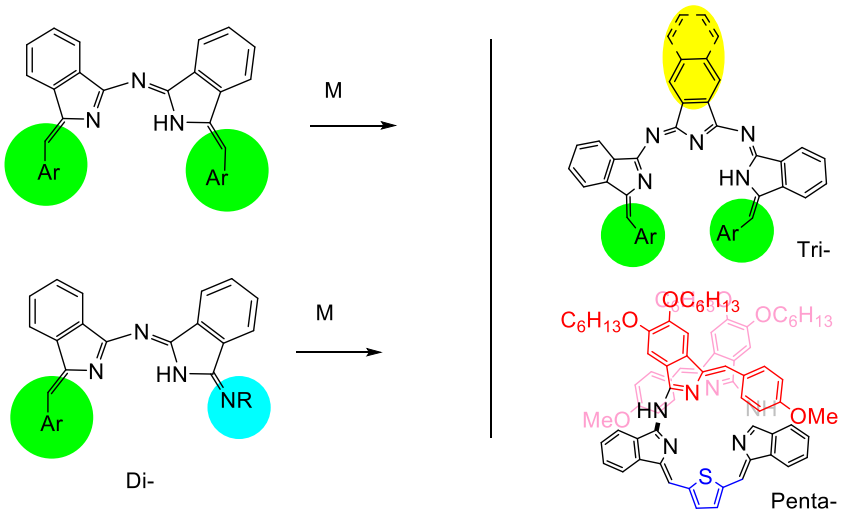
Aza-Dipyrromethene and Aza-BODIPY analogues; extended systems and diverse complexation chemistry

Andrew N. Cammidge[a], **Isabelle Chambrier, Bandar Alshammari, Aishah Alzahrani, Ibtesam Mashnoy, David L. Hughes**

[a]*School of Chemistry, Pharmacy and Pharmacology, University of East Anglia, Norwich Research Park, Norwich NR4 7TJ. United Kingdom.*

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Benzo-fused analogues of aza-DPMs and aza-BODIPYs have a different electronic configuration compared to normal (aza) DPMs/BODIPYs but share their interesting properties and versatility [1, 2]. Here, we summarise and extend the synthesis strategies for this family of aza-DPMs, aza-BODIPYs, and trimer systems. The complexation chemistry of these ligands is diverse and intriguing. In many cases, this leads to stable complexes, whereas in other cases, the outcomes include higher-order analogues (dimerization of dimers) and even macrocyclization. Linear systems, such as pentamers, can be assembled through sequential, controlled syntheses.



REFERENCES

1. A. Diaz-Moscoso, E. Emond, D. L. Hughes, G. J. Tizzard, S. J. Coles and A. N. Cammidge "Synthesis of a class of core-modified Aza-BODIY derivatives" *J. Org. Chem.* **79**, 8932-8936, 2014. DOI 10.1021/jo501863t.
2. B. N. Alanazi, A. O. Alsahli, S. Remiro-Buenamanana, A. Diaz-Moscoso, F. H. Alkorbi, N. A. Alsaiari, C. Marrett-Munro, I. Chambrier, D. L. Hughes, G. J. Tizzard, S. J. Coles and A. N. Cammidge "A Family of Symmetrical and Unsymmetrical Aza-Dipyrromethenes and Aza-BODIPYs with Through-Bond and Face-To-Face π-Interaction between Termini" . *Chem. Eur. J.* **31**, e202501862, 2025.

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Synthesis of Planar and Curved π-Extended Anthracenyl Porphyrins by On-Surface Cyclodehydrogenation

Stéphane Campidelli[a], **Joffrey Pijeat**[a], **Karl-Heinz Ernst**[b], **Miloš Baljozović**[b]

[a]*Université Paris-Saclay, CEA, CNRS, NIMBE, LICSEN, 91191 Gif-sur-Yvette, France.*
[b]*Molecular Surface Science Group, Empa, 8600 Dübendorf, Switzerland.*

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For the last fifteen years, on-surface synthesis became an extremely popular and powerful method to fabricate nanostructures which otherwise would not have been accessible by conventional wet organic syntheses. The syntheses, realized in the chamber of high vacuum scanning tunneling microscope (STM), permitted the fabrication and the characterization of atomically defined nanostructures such as polycyclic aromatic hydrocarbons (PAH), graphene nanoribbons or 2D covalent networks.[1] Among the organic molecules studied by STM, porphyrins are of particular importance because of their electronic and optical properties. Initial studies were mainly devoted to the supramolecular organization of porphyrins and porphyrin derivatives on surface and it is only in 2007 that noble metal surfaces were used as catalytic surface to perform reactions on the porphyrin.[2] Since then, examples of open-shell porphyrin derivatives[3] and conjugated oligomers.[4] were reported.
Herein, we report an *in vacuo* temperature controlled cyclodehydrogenation of bis- and tetra-anthracenyl Zn(II) porphyrins on a gold(111) surface.[5] By gradually increasing the temperature, sequential dehydrogenation leads to the formation of fused anthracenyl porphyrin products. Notably, at high molecular coverage, the formation of bowl-shaped porphyrins occurs. These findings open the door to a variety of π-extended anthracenyl-containing porphyrin products *via* cyclodehydrogenation and transmetalation, offering significant potential in the fields of molecular (photo/electro)catalysis, (opto)electronics, and spintronics (Figure 1).

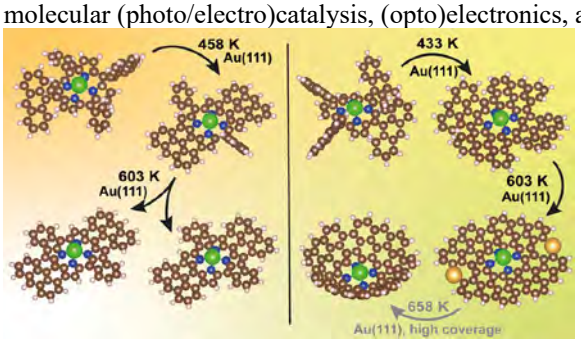


Figure 1. Schematic representation of the "on-surface" synthesis of π-extended anthracenyl porphyrin derivatives.

REFERENCES

1. Clair S, de Oteyza DG. *Chem. Rev.* 2019; **119**: 4717−4776.
2. Grill L, Dyer M, Lafferentz L, Persson M, Peters MV, Hecht S. *Nat.Nanotechnol.* 2007; **2**: 687−691.
3. a) Sun Q, Mateo LM, Robles R, Ruffieux P, Lorente N, Bottari G, Torres T, Fasel R. *J. Am. Chem. Soc.* 2020; **142**: 18109−18117; b) Zhao Y, Jiang K, Li C, Liu Y, Xu C, Zheng W, Guan D, Li Y, Zheng H, Liu C, Luo W, Jia J, Zhuang X, Wang S. *J. Am. Chem. Soc.* 2020; **142**: 18532−18540.
4. a) Mateo LM, Sun Q, Liu SX, Bergkamp JJ, Eimre K, Pignedoli CA, Ruffieux P, Decurtins S, Bottari G, Fasel R, Torres T. *Angew. Chem. Int. Ed.* 2020; **59**: 1334−1339; b) Mateo LM, Sun Q, Eimre K, Pignedoli CA, Torres T, Fasel R, Bottari G. *Chem. Sci.* 2021; **12**; 247−252.
5. Baljozović M, Pijeat J, Campidelli S, Ernst KH. *J. Am. Chem. Soc.* 2024; **146**: 34600−34608.

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Perfluorinated Zinc Porphyrin for Sensitized Photoelectrosynthetic Cells

Stefano Caramori[a], Edoardo Marchini[a], Francesca Tessore[b], Gabriele di Carlo[b]

[a]*Department of Chemical, Pharmaceutical and Agricultural Sciences of the University of Ferrara, Via Luigi Borsari 46, 44121, Ferrara, Italy*
[b]*Deparment of Chemistry, University of Milan, Via Golgi 19, 20133 Milan, Italy*

This study reports about a series of perfluorinated Zn(II) porphyrins designed as sensitizers for photoelectrosynthetic cells, [1-4] with a focus on promoting the oxidation of benzyl alcohol (BzOH) mediated by the 2,2,6,6-tetramethyl-1-piperidine N-oxyl (TEMPO) organocatalyst. Three dyes, CLICK-3, CLICK-4, and BETA-4, are meticulously designed to explore the impact of substituents and their positions on the perfluorinated porphyrin ring in terms of redox potentials and energy level alignment when coupled with SnO_2/TiO_2-based photoanodes and TEMPO mediator. A comprehensive analysis utilizing spectroscopy, electrochemistry, photophysics, and computational techniques of the dyes in solution and sensitized thin films unveils an enhanced charge-separation character in the 4D−π–1A type BETA-4. Incorporating four dimethylamino donor groups at the periphery of the porphyrin ring and a BTD-accepting linker at the β-pyrrolic position equips the structure with a more efficient donor–acceptor system. This enhancement ensures improved light-harvesting capacity, resulting in a doubled incident photon-to-current conversion efficiency (IPCE% ≃30%) in the presence of LiI compared to meso-substituted dyes CLICK-3 and CLICK-4. Sensitizing SnO_2/TiO_2 thin films with BETA-4 successfully promotes the photooxidation of benzyl alcohol (BzOH) in the presence of the rapid TEMPO [5] radical catalyst, yielding photocurrents of approximately 125 μA/cm^2 in an optimized TBPy/$LiClO_4$/ACN electrolyte. Notably, when lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) replaces TBPy as the base for TEMPO-catalyzed BzOH oxidation, a remarkable photocurrent of around 800 μA/cm2 is achieved, marking one of the highest values reported for this photoelectrochemical reaction to date. This study underscores that the proper functionalization of perfluorinated zinc porphyrins positions these dyes as ideal candidates for sensitizing SnO_2/TiO_2 in the photodriven oxidation of BzOH. It also highlights the crucial role of carefully tuning electrolyte composition based on the electronic properties of molecular sensitizers.

REFERENCES

1. G. di Carlo et al. ACS Appl. Mater. Interfaces 2024, 16, 12, 14864–14882
2. A. Orbelli Biroli et al. ACS Appl. Mater. Interfaces 2019, 11, 36, 32895–32908
3. H. Imahori Bull. Chem. Soc. Jpn. 2023, 96, 339– 352,
4. Y. Zhou et al. J. Am. Chem. Soc. 2024, 146, 31, 21903–21912
5. E. Nikoloudakis et al. ACS Catal. 2021, 11, 19, 12075–12086

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Solar-Driven Photocatalysis for Hydrogen Production and Carbon Dioxide Conversion

Georgios Charalambidis[a], Fabrice Odobel[b], Athanassios G. Coutsolelos[c,d]

[a]*Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, 11635 Athens, Greece.*
[b]*Université de Nantes, CNRS, Chimie et Interdisciplinarité: Synthèse, Analyse, Modélisation (CEISAM), UMR 6230, 2 rue de la Houssinière 44322, Nantes, France.*
[c]*Laboratory of Bioinorganic Chemistry, Department of Chemistry,University of Crete, Voutes Campus, 70013, Heraklion, Crete, Greece.*
[d]*Institute of Electronic Structure and Laser (IESL) Foundation for Research and Technology - Hellas (FORTH), Vassilika Vouton, GR 70013 Heraklion, Crete, Greece.*

The persistent global dependence on fossil fuels has led to severe environmental challenges, largely driven by the rapid rise in greenhouse gas emissions. Developing cost-competitive, low-carbon technologies based on renewable energy is therefore essential. Among all renewable sources, solar energy holds the highest potential for large-scale sustainable deployment. Hydrogen, a zero-emission energy carrier, represents an attractive alternative to carbon-based fuels, particularly when produced photocatalytically from water. Likewise, the photocatalytic conversion of CO_2 into value-added chemical fuels offers a promising route to both mitigate emissions and generate useful products. Inspired by natural photosynthesis, a wide range of artificial photocatalytic systems based on porphyrinoids have been designed and evaluated over the last years.[1]

In this presentation, I will discuss our recent progress in the development of photocatalytic systems for hydrogen evolution and CO_2 reduction that employ porphyrin derivatives as chromophores or as molecular catalysts. I will highlight our advances in heterogeneous photocatalysis, including the use of self-assembled supramolecular porphyrinoid nanostructures[2] and dye-sensitized photocatalytic systems (DSPs).[3] Finally, I will address our efforts to improve the overall sustainability of these processes by replacing conventional sacrificial electron donors with productive oxidation reactions, specifically the photocatalytic oxidation of alcohol derivatives.[4]

REFERENCES

1. E. Nikoloudakis, I. López-Duarte, G. Charalambidis, K. Ladomenou, M. Ince, A.G. Coutsolelos, *Chem. Soc. Rev.*, **2022**, *51*, 6965.
2. E. Triantafyllou, E. Nikoloudakis, S. Psilodimitrakopoulos, D. Kavalieros, G. Landrou, E. Stratakis, G. Charalambidis, A. Mitraki, A.G. Coutsolelos, *ChemSusChem*, **2025**, *18*, e202501251.
3. V. Nikolaou, E. Nikoloudakis, G. Charalambidis, A. G. Coutsolelos, *Chem. Commun.*, **2025**, *61*, 10086.
4. D. Romito, C. Govind, V. Nikolaou, R.J. Fernández-Terán, A. Stoumpidi, E. Agapaki, G. Charalambidis, S. Diring, E. Vauthey, A.G. Coutsolelos, F. Odobel, *Angew. Chem. Int. Ed.*, **2024**, *63*, e202318868.

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Advanced Porphyrin Nanoparticles for Cancer Theranostics

Juan Chen[a], **Gang Zheng**[b]

[a] *Princess Margaret Cancer Centre, University Health Network, Toronto, Canada*
[b] *Department of Medical Biophysics, University of Toronto, Toronto, Canada*

Photodynamic therapy (PDT) utilizes light-activated photosensitizers to generate cytotoxic reactive oxygen species for localized tumor ablation. To improve treatment selectivity and reduce off-target effects, we pioneered a concept of activatable photosensitizers, in which photodynamic activity remains quenched until activated by disease-specific interactions [1]. Building on this concept, we developed porphysomes—liposome-like nanostructures self-assembled from porphyrin-lipid conjugates—that circulate in a photophysically quenched state and recover fluorescence and PDT activity upon cellular uptake and nanostructure disassembly. Porphysomes enable multimodal imaging and therapeutic applications, including photoacoustic imaging, photothermal therapy, positron emission tomography (PET), fluorescence imaging and PDT, and are now progressing toward clinical translation. To further improve translational potential and improved PDT efficacy, we developed PEG-free, ultrasmall porphyrin lipoprotein–like particles (PLP) that mimic the structure and function of high-density lipoproteins (HDL). These theranostic nanostructures integrate PET, fluorescence imaging, and activatable PDT within a single HDL-like platform and exhibit favorable pharmacokinetics without PEGylation. Rapid intracellular trafficking and dissociation of PLP within tumors restore porphyrin fluorescence and photodynamic activity, enabling low-background imaging and efficient PDT [2]. To address the unique challenges of glioblastoma (GBM), including blood–brain barrier penetration and heterogeneous intratumoral delivery, PLP was further engineered with a single apolipoprotein E–mimetic peptide [3]. This design promotes stable HDL-like assembly while enabling multivalent engagement of LDLR, LRP-1, and SR-B1, resulting in enhanced porphyrin delivery and improved PDT efficacy in GBM models. Finally, to overcome hypoxia-associated limitations of PDT, we developed a perfluorocarbon nanoemulsion incorporating a porphyrin–lipid conjugate, which enhances oxygen availability and achieves potent PDT responses in lung cancer models. Collectively, these advanced porphyrin-based nanoplatforms provide a versatile and clinically translatable framework for multimodal cancer imaging and therapy in challenging disease settings.

REFERENCES

1. Chen J, Stefflova K, Niedra M, Wilson BC, Chance B, Glickson JD, Zheng G, Protease-Triggered Photosensitizing Beacon Based on Singlet Oxygen Quenching and Activation. JACS, 2004, 126, 11450~1.
2. Cui LY, Tokarz D, Cisek R, Ng KK, Wang F, Chen J, Barzda V, Zheng G, Organized Aggregation of Porphyrins in Lipid Bilayer for Third Harmonic Microscopy. Angew Chem Int Ed Engl, 2015, 54: 13928-13932.
3. Datta G, Chaddha M, Garber DW, Chung BH, Tytler EM, Dashti N, Bradley WA, Gianturco SH, Anantharamaiah, GM, The Receptor Binding Domain of Apolipoprotein E, Linked to a Model Class A Amphipathic Helix, Enhances Internalization and Degradation of LDL by Fibroblasts. Biochemistry 2000, 39 (1), 213–220.

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Red-shifted chlorophylls and their containing organisms: Current status

Min Chen

School of Life and Environmental Sciences, The University of Sydney, Australia. E-mail: min.chen@sydney.edu.au

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Chlorophyll *d* and chlorophyll *f* are red-shifted chlorophylls, because their Q absorption bands are significantly red-shifted compared to chlorophyll *a*. The discovery of chlorophyll *f* in 2010 [1] and the subsequent characterization of chlorophyll *f*-containing cyanobacteria [2, 3] have led to new research directions, opened new avenues, and challenged the physical limits of oxygenic photosynthesis [4-6]. In my presentation, I will report on the chemistry and function of red-shifted chlorophylls and introduce the potential application of such profound consequences on their red-shifted electronic absorption spectra in photosynthesis and beyond [7-10], including the unique adaptations that have allowed the proliferation of chlorophyll *d*- and chlorophyll *f*-containing organisms in diverse ecological niches around the world.

REFERENCES

1. Chen M, Schliep M, Willows R, Cai Z-L, Neilan BA and Scheer H (2010) *Science* 329:1318–1319.
2. Chen M, Li Yaqiong, Birch D, Willows RD (2012) *FEBS Lett.*586:3249–3254.
3. Zhang Z-C, Li Z-K, Yin YC, Li Yq, Jia Y, Chen M and Qiu B-S (2019) . *Environ microbiol*. 21:1497-1510.
4. Chen M and Blankenship RB (2011) *Trends in Plant Science* 16:427–431.
5. Chen M and Scheer H (2013) *Journal of Porphyrins and Phthalocyanines* 17:1–15.
6. Chen M (2014) *Annual Review of Biochemistry* 83:317–340.
7. Li Y, Cai Z-L and Chen M (2013) *J. Phys. Chem. B* 117:11309–11317.
8. Schmitt F J, et al, (2019) *Photosyn.Res* 139: 185-201.
9. Sawicki A, Willows RD and Chen M (2019) *Photosyn. Res*, 140(1):115-127.
10. Chen M, Hernandez-Prieto MA, Loughlin PC, Li Yq and Willows RD (2019) BMC genomics 20 (1), 207.

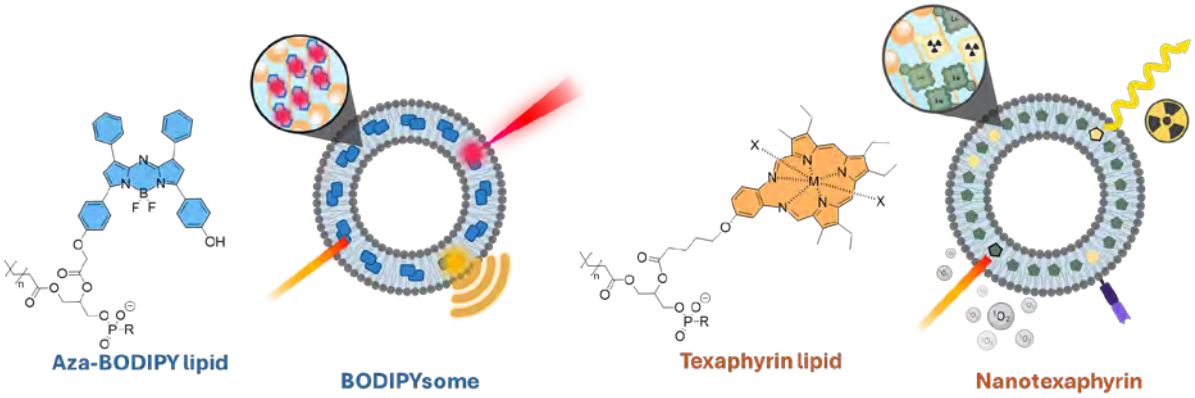
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Porphyrinoid Nanomedicines for Advanced Theranostics

Miffy Hok Yan Cheng[a]

[a] *Faculty of Pharmaceutical Sciences, 2405 Wesbrook Mall, Vancouver, British Columbia V6T 1Z3, Canada*



Porphyrinoids such as BODIPY and texaphyrin are powerful photochemical agents for photodynamic therapy (PDT), as well as radio- and fluorescence-based imaging, making them potential candidates for diagnosis and therapy ("theranostics"). However, their clinical translation is often limited by poor bioavailability and the lack of intrinsic targeting capabilities. Lipid-based nanoparticles offer an effective strategy to address these limitations in cancer nanomedicine. In this presentation, we describe a "one-for-all" liposomal formulation strategy that integrates novel organic chromophores (aza-BODIPY and texaphyrin) to enable multimodal imaging and theranostic properties. First, we describe the development of BODIPYsomes, formed from aza-BODIPY lipids, which exhibit nanoconfinement-induced optical properties enabling high-contrast, dual-modality tumour imaging [1]. Second, we present the development of metallonanotexaphyrins, texaphyrin-based nanoparticles that chelate both "hot" and "cold" trivalent metals to generate PSMA-^{111}In/Lu-nanotexaphyrins for tumour targeting, SPECT/CT, and PDT [2], as well as myoglobin-loaded ^{177}Lu/Gd-nanotexaphyrins for radiotherapy, SPECT/CT, and MRI. These examples demonstrate image-guided therapy with real-time tracking. Finally, we discuss emerging opportunities and remaining challenges associated with the radiolabelling of ^{201}Tl-based nanotexaphyrins, and highlights the need for continued investigation into porphyrinoid chemistry for biological and clinical applications.

REFERENCES

1. M. H. Y. Cheng, K. M. Harmatys, D. M. Charron, J. Chen, G. Zheng, *Angew. Chem. Int. Ed.* **2019**, *58*, 13394.
2. M. H. Y. Cheng, M. Overchuk, M. A. Rajora, J. W. H. Lou, Y. Chen, M. G. Pomper, J. Chen, and G. Zheng, *Molecular Pharmaceutics* **2022** *19* (6), 1803-1813
3. X. Ma, X. Liang, M. Yao, Y. Gao, Q. Luo, X. Li, Y. Yu, Y. Sun, M. H. Y. Cheng, J. Chen, G. Zheng, J. Shi, F. Wang. *Nat Commun* **2023**, 14, 6187.
4. K M. Wulfmeier, M. H. Y. Cheng, Z. Cai, S. Y. A. Terry, V. Abbate, P. J. Blower, G. Zheng, and R. M. Reilly *Molecular Pharmaceutics* **2025,** 22 (1), 242-254

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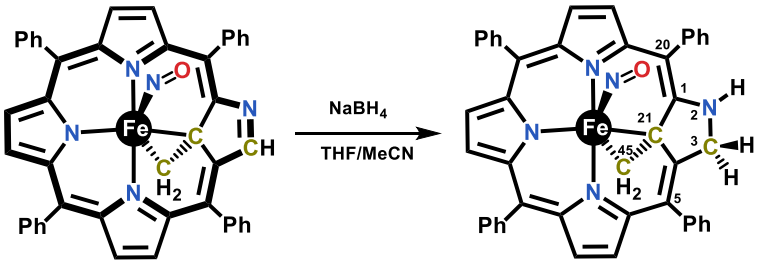


Regioselective reduction of N-confused porphyrin: N-Confused Chlorin iron nitrosyl complex

Wei-Min Ching*[a], Cheng-Chau Chiu*[b], Chen-Hsiung Hung[c]

[a]*Department of Chemistry, National Kaohsiung Normal University, Kaohsiung 82444, Taiwan*
[b]*Department of Chemistry, National Sun Yat-sen University, Kaohsiung 804201, Taiwan*
[c]*Institute of Chemistry, Academia Sinica, Taipei 115, Taiwan*

Treating the reductant with [Fe(CTPPCH_2)NO] [1-2] leads to the formation of an unexpected N-confused chlorin iron nitrosyl complex, [Fe(CTPPCH_2-Chlorin)NO], rather than the NC-phlorin [3] or other reduced iron nitrosyl complexes. The UV-vis spectrum shows a Soret band at 364 nm, distinct from the 460 nm band of [Fe(CTPPCH2)NO]. Although the crystal structures of [Fe(CTPPCH_2-Chlorin)NO] and [Fe(CTPPCH2)NO] are similar, the ^{1}H-NMR spectrum indicates an incomplete pi-conjugate system characteristic of N-confused porphyrin. This is notably different from the starting complex, [Fe(CTPPCH_2)NO]. The IR and ^{15}N-NMR spectra also suggest a significant NO radical character in [Fe(CTPPCH_2-Chlorin)NO], closely resembling [Fe(CTPPCH_2)NO] and [Fe(*H*CTPPCH_2)NO]$^+$. To identify the N-confused chlorin structure and the location of the extra proton, methods such as deuterium substitution of four benzene groups, deuterium substitution of the methylene group in [Fe(CTPPCH_2)NO], complete 2D NMR analysis, reaction with $NaBD_4$, and DFT calculation are employed. The analysis indicates that the reduction of [Fe(CTPPCH_2)NO] occurs through a regioselective reduction of N-confused porphyrin, resulting in the formation of [Fe(CTPPCH_2-Chlorin)NO].



REFERENCES

1. *Dalton Trans.*, **2017**, 46, 15087–15094
2. *Chem. Commun.*, **2012**, 48, 4989–4991
3. *J. Porphyrins Phthalocyanines* **2014**, *18*, 909–918.

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Exploring the Chemistry of 1,7-Naphthiporphyrin Derivatives through a Molecular Engineering Approach

Dong-Gyu Cho

Department of Chemistry and Chemical Engineering, Inha University, Incheon 22212, Republic of Korea

Since the discovery of 1,7-naphthiporphyrin (**1**),[1] we have systematically modified its core structure.[2] Truncation of the naphthalene unit and the use of regioisomeric forms of 1,7-naphthalene enabled the synthesis of allyliporphyrin (**2**) and 1,2- (2,3- or 3,4-) naphthiporphyrins **(3**, **4**, and **5**), respectively. These unique structures were deliberately designed to address important scientific questions, such as whether electron-withdrawing or electron-donating groups on benzene rings or large aromatic macrocycles can reduce their intrinsic aromaticity,[3] and whether Clar's sextet model can be reconciled with resonance theory.[4] These issues are discussed in detail.

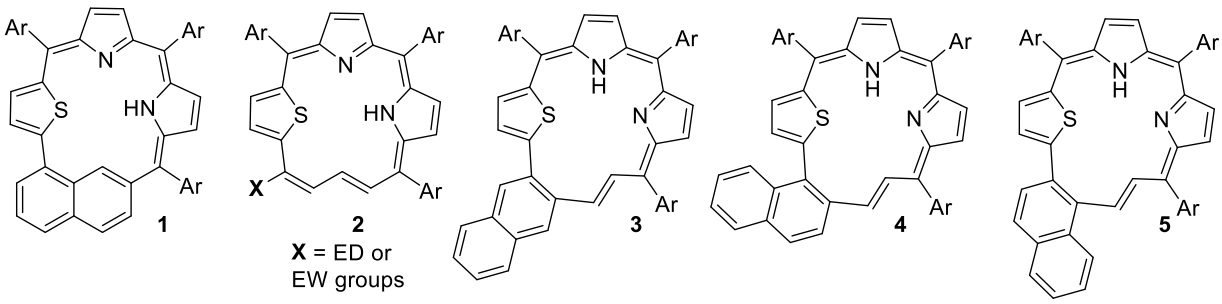


Figure 1. 1,7-naphthiporphyrin and their derivatives

REFERENCES

1. Hong, J.-H.; Aslam, A. S.; Ishida, M.; Mori, S.; Furuta, H.*; Cho, D.-G.* *J. Am. Chem. Soc.* **2016,** *138* (15), 4992-4995.
2. Ko, M.-S.; Cho, D.-G.* *Acc. Chem. Res.* **2025**, *58* (15), 2425-2439.
3. Ko, M.-S.; Roh, T.-H.; Desale, P. P.; Choi, S.-W.; Cho, D.-G.* Effects of Electron-Withdrawing and Electron-Donating Groups on Aromaticity in Cyclic Conjugated Polyenes. *J Am Chem Soc* **2024**, *146* (9), 6266-6273.
4 Desale, P. P.; Ko, M.-S.; Roh, T.-H.; Ham, J.-I.; Cho, D.-G.* *J. Am. Chem. Soc.* **2025**, *147* (1), 480-487.

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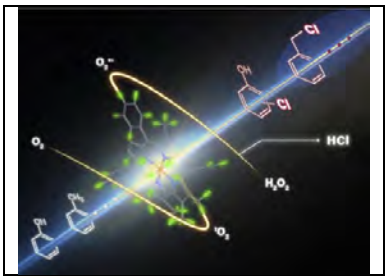


Enabling Dual C–H Chlorination and H_2O_2 Generation with CF_3-containing Phosphorus Corroles

David G. Churchill[a,b], Xuan Zhan[c], Donghyeon Kim[d], Zakir Ullah[e],

[a] *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea. dchurchill@kaist.ac.kr.* [b] *KAIST Institute for Health Science and Technology (KIHST) (Therapeutic Bioengineering Section), Daejeon 34141, Republic of Korea.* [c]*School of Chemical Engineering and Technology, Sun Yat-sen University, Zhuhai 519082, China.* [d]*Center for Advanced Reaction Dynamics, Institute for Basic Science (IBS), Daejeon 34141, Republic of Korea.* [e]*Institut de Ciència de Materials de Barcelona (ICMAB–CSIC), Consejo Superior de Investigaciones Científicas, Campus Universitari de Bellaterra, Cerdanyola del Vallès 08193, Spain.*

The efficient photocatalytic chlorination of aromatics was achieved using a P–corrole derivative. In particular, dual catalysis was observed in both chlorination and H_2O_2 formation. We have found that reproducibility and stability of these experiments holds over multiple cycles, highlighting its practical utility. The corrole photocatalyst in question is the highly oxidizing penta–beta-CF_3 substituted 2,3,8,17,18–pentatrifluoromethyl–(5,10,15–tris(pentafluorophenyl) corrole phosphorus (V) difluoride). P–(CF3)5 showed efficacy in the chlorination of phenol and related natural compounds. Simultaneous photocatalytic chlorination of phenol or toluene and H_2O_2 formation was achieved, with the latter achieving a notable rate of > 7 mM/g/h under ambient conditions. Notably, the oxidation of toluene predominantly yields benzaldehyde over benzyl chloride. The H_2O_2 formation can be tuned by adjusting the water/acetonitrile ratio as well as via acid concentration. Comprehensive experimental and theoretical (DFT) investigations were conducted to elucidate the underlying mechanisms of both chlorination and oxidation. This dual–function corrole demonstrates the potential of non–precious main group systems as viable stable photocatalysts. The catalytic process not only enhances reaction efficiency but also underscores the potential of corrole–based catalysts in advancing sustainable and green chemical methodologies. This presentation will also include sufficient background about synthesis, structure, and related earlier reported bromination studies.



REFERENCES

1. Zhan, X., Kim, D., Ullah, Z., Churchill, D. G. « Corrole–chelated phosphorus complex: enabling dual C–H chlorination and H_2O_2 generation. » *Journal of Molecular Liquids* **2024**, 413, 125938.
2. Zhan, X.; Teplitzky, P.; Diskin–Posner, Y.; Sundararajan, M.; Ullah, Z.; Chen, Q.–C.; Shimon, L. J. W.; Saltsman, I.; Mahammed, A.; Kosa, M.; Baik, M.-H., Churchill, D. G., Gross, Z. « Maximizing Property Tuning of Phosphorus Corrole Photocatalysts through a Trifluoromethylation Approach. » *Inorg. Chem.* **2019**, 58 (9), 6184–6198.
3. Lee, W., Zhan, X., Palma, J., Vestfrid, J., Gross, Z., & Churchill, D. G. « Minding our P-block and Q-bands: paving inroads into main group corrole research to help instil broader potential. » *Chemical Communications*, **2021**, 57(38), 4605-4641.

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Porphyrine-based conjugated polyHIPEs for photocatalytic degradation of organic pollutants

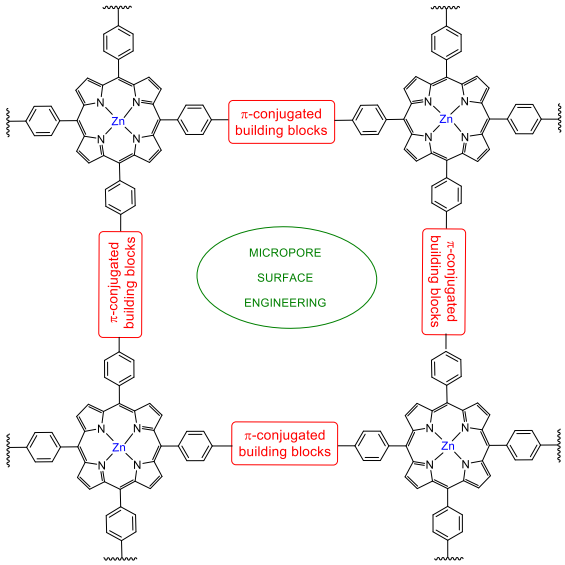
Sébastien Clément[a], **Julie-Lisa Malaval**[a], **Michel Granier**[a], **Sébastien Richeter**[a]

[a] *ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier, France.*

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Conjugated polyHIPEs are lightweight, highly porous organic materials synthesized via the polymerization of high internal phase emulsions (HIPEs), typically using metal-catalyzed cross-coupling reactions.[1-2] Their remarkable properties arise from their unique hierarchically interconnected 3D architecture, composed of micrometer-sized macropores, submicrometer windows, and frequently meso- and micropores within the polymer walls. [3] Beyond their structural advantages, their extended π-conjugated framework imparts semiconducting behavior, strong absorption in the visible region, and tunable band gaps — making them particularly attractive for photocatalytic applications. [3]

In this work, we report the synthesis of porphyrin-based conjugated polyHIPEs prepared via Suzuki cross-coupling. Porphyrin building act as photosensitizers within the network, while thermocleavable groups were strategically introduced as spacers inside the microporous framework to enable post-synthetic modulation of the internal surface chemistry. Their ability to generate singlet oxygen were exploited as reusable photocatalysts for degradation of pollutants such as rhodamine B.



REFERENCES

1. Z. Jun Wang, S. Ghasimi, K. Landfester, K. A. I. Zhang, *Chem. Commun.* **2014**, *50*, 8177.
2. T. Kotnik, G. Žerjav, A. Pintar, E. Žagar, S. Kovačič, *Polym. Chem.* **2022**, *13*, 474.
3. J.-L. Malaval, M. Granier, P. Gerbier, S. Richeter, S. Clément, *Polymer Int.* **2026**, *In press*. https://doi.org/10.1002/pi.70042

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Caged Metallocorrole Complexes : getting closure to metalloenzymes' functionalities.

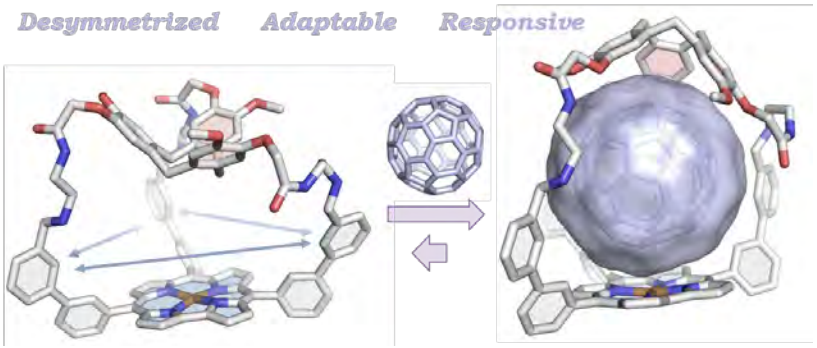
A. Baidiuk,[a] X. Ribas, [b] M. Orio, [a] A. Martinez, [a] G. Canard, [c] Cédric Colomban [a]

[a] *iSm2, UMR-7313, Aix-Marseille Univ., CNRS, Marseille, France*
[b] *IQCC, Departament de Quimica. Universitat de Girona, Catalonia, Spain*
[c] *CINaM, UMR-7225, Aix Marseille Univ., CNRS, Marseille, France*

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We develop metalloprotein-inspired metal complexes entrapped in chiral artificial cages enabling advanced catalysts (eg CH_4 oxidation), and receptors.[1] These caged metal complexes have been studied as catalysts for O_2 reduction reactions, and oxidations of C-H bonds by high-valent metal-O_2 intermediates.[2]
In this context, metallocorroles have recently emerged as a promising class of redox-active catalysts displaying distinct reactivity and selectivity compared to the time-honored porphyrin catalysts.[3] However, unlike widely studied porphyrin-based cages, no example of a metallocorrole cage has been reported so far, presumably due to difficult preparation.

Herein, we introduce a new design of heme-like cages based on corroles, the desymmetrized analogue of metalloporphyrins. Theses unprecedented metallocorrole cages aims at developing *i*) advanced receptors allowing binding of electroactive fullerenes guests in a guest-adaptive, stimuli-responsive and low-symmetry cavity, [4] and *ii*) confined redox-active Co(III) and Cu(III) corrole catalysts. The designed strategy being generalizable across the formation of various corrole cages, it provides basis for development of a new class of low-symmetrical heme-like receptors and opens valuable perspectives in the field of catalysis in confined space.



Discussion on *i*) the synthetical keys allowing to unlock the preparation of the first metallocorrole cage, ii) how the conformationaly adaptive mettalocorrole cage could reversibly bind fullerenes in a chiral, stimuli-responsive and low-symmetry cavity, and iii) how the cage could be used to reach selective functionalization of electroactive fullerene guests, will be the core of this communication, which aims at establishing a key precedent of one artificial caged complex regrouping several key features of metalloproteins.

REFERENCES

1. D. Diao, … , C. Colomban, *Chem.Commun.* **2023**, 59, 4288, *Emerging investigators collection*.
2. D. Diao, A. Baidiuk … , C. Colomban, *JACS-Au*. **2024**, 4, 1966.
3. C. Di Natale, C. Gros, R. Paolesse, *Chem. Soc. Rev.* **2022**, 51, 1277–1335
4. A. Baidiuk, … , G. Canard, C. Colomban, *ChemRxiv.* **2025** (10.26434/chemrxiv-2025-lprmp)

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Self-modulation and Self-protection Mechanisms in Molecular Catalysis of Electrochemical Reactions

Cyrille Costentin[a]

[a] *Univ Grenoble Alpes, DCM, CNRS, 38000 Grenoble, France*

Molecular catalysis of electrochemical reactions is a rapidly evolving field, with significant emphasis on small molecule activation and the electrification of chemical transformations. Gaining mechanistic insight is crucial for the rational design of more efficient catalysts and processes. In this context, we will present recent advances in the mechanistic analysis of molecular electrochemical catalysis.
First, we will demonstrate how a transition metal complex can undergo self-modulation due to the generation of a strongly coordinating ligand. This concept will be introduced and exemplified by the catalytic reduction of N_2O to N_2 by iron porphyrins [1] as well as CO_2 reduction by a cobalt macrocyclic ligand. [2]
Second, we will explore the role of O_2 in the molecular catalysis of CO_2 reduction, where achieving O_2 tolerance remains a key challenge for practical applications. We will reveal a self-protection mechanism that emerges when suitable transition metal complexes are employed as catalysts, illustrated by the CO_2-to-CO conversion catalyzed by iron porphyrins. [3]

REFERENCES

1. Chartier, C.; Deeba, R.; Collard, A.; Chardon-Noblat, S.; Costentin, C. *ACS Catal.* **2024**, *14*, 14509-14516.
2. Harvey, M. C.; Chardon-Noblat, S.; Costentin, C. *J. Am. Chem. Soc.* **2025**, *147*, 24171-24178
3. Feldman, D. M.; Julliard, P.-G.; Madrigalejo, J.-C.; Fortage, J.; Collomb, M.-N.; Costentin, C. *J. Am. Chem. Soc.* **2026**, *DOI : 10.1021/jacs.5c19804*

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The pigments of life: A continuous source of inspiration for new materials and applications

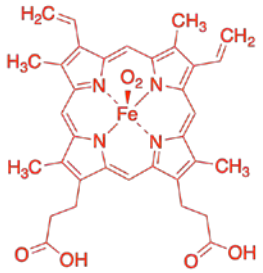
Athanassios G. Coutsolelos, Emmanuel Stratakis

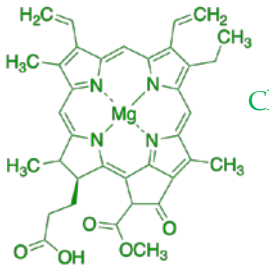
Department of Chemistry, University of Crete, Laboratory of Bioinorganic Chemistry, Voutes Campus, 70013 Heraklion, Crete, Greece. (e-mail: acoutsol@uoc.gr)
Institute of Electronic Structure and Laser (I.E.S.L.) Foundation for Research and Technology-Hellas (FO.R.T.H.), Vassilika Vouton, 70013, Heraklion, Crete, Greece.

ORALS

Natural photosynthetic processes have increasingly inspired the fabrication of nanostructured molecular materials with advanced light-harvesting and electron-transfer properties. [1-6] In this context, supramolecular chemistry allows diverse and disparate molecular building blocks to be amalgamated into highly ordered architectures. These mimic the key functions of the photosynthetic reaction center: light harvesting, charge separation, charge transport, energy transfer, and catalysis. [7,8] Porphyrinoids, the basic building block of chlorophylls, have emerged as an exceptional class of light harvesters and electron donors in such supramolecular electron donor-acceptor hybrids [9-12]. A variety of applications, from solar cells to hydrogen production to medicine, were reported.

Heme





Chlorophyll

REFERENCES

1. M. R. Wasielewski, *Chem. Rev.*, 1992, **92**, 435-461.
2. R. E. Blankenship, *Molecular Mechanisms of Photosynthesis*, Blackwell Science, Oxford, U.K., 2002.
3. D. Gust, T. A. Moore and A. L. Moore, *Acc. Chem. Res.*, 1993, **26**, 198-205.
4. H. B. Gray and J. R. Winkler, *Annu. Rev. Biochem.*, 1996, **65**, 537-561.
5. M. Grätzel, *Journal of Photochemistry and Photobiology C: Photochemistry Reviews*, 2003, **4**, 145-153.
6. T. Nakanishi, *Supramolecular Soft Matter, Applications in Materials and Organic Electronics*, John Wiley &Sons, New Jersey, 2011.
7. D. M. Guldi, *Chem. Soc. Rev.*, 2002, **31**, 22-36.
8. F. D'Souza, *Handbook of Carbon Nanomaterials, Synthesis and Supramolecular Systems*, World Scientific Publishing Co. Pte. Ltd, Singapore, 2011.
9. Manas K. Panda, Kalliopi Ladomenou, and Athanassios G. Coutsolelos, Coordination Chemistry Reviews **21-22**, 2601-2627.
10. K. Ladomenou, M. Natali, E. Iengo, F. Scandola, G. Charalampidis, A. G. Coutsolelos *Coordination Chemistry Reviews*, 2015, 38-54.
11. C. Stangel, C. Schubert, S. Kuhri, G. Rotas, J.T. Margraf, E. Regulska, T. Clark, T. Torres, N. Tagmatarchis, A. G. Coutsolelos, D. M. Guldi. *Nanoscale* 2015, **7**, 2597-2608.
12. V. Nikolaou, K. Ladomenou, G. Charalambidis, A. G. Coutsolelos, *Coordination Chemistry Reviews*, 2016, 1-42.

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Exploiting porphyrins to induce antiparallel to parallel transition of RNA G-quadruplex

Alessandro D'Urso[a],

[a]*University of Catania, Chemical Science Department, Viale A. Doria 6, 95125 Catania, Italy.* adurso@unict.it

The human genome is a complex mosaic of sequences with different functionality, among which telomeric repeat containing RNA (TERRA), a guanine-rich sequence, holds a unique place due to its pivotal role in maintaining genomic integrity.[1] Telomeric RNA can adopt a four-stranded G-quadruplex (G4) conformation where the 2′ hydroxyl group in ribose sugars enhances RNA G4 stability by promoting more intramolecular interactions within the structure. Specifically, these hydroxyl groups impose significant conformational constraints, effectively hindering the G4 from adopting a syn-conformation, which is necessary for an antiparallel topology.[2] However, recent studies [3,4] have revealed the formation of an intramolecular antiparallel G4 formed by human telomere RNA, demonstrating that RNA G4s have the capacity to exhibit polymorphism, assuming configurations distinct from the parallel arrangement. In this context, designing specific ligands capable to interact with these G4 structures is helpful for studying their conformations and inhibiting telomerase enzyme activity as a potential anticancer therapy.

Porphyrins are hetero-aromatic macrocycles present remarkable electronic properties which bring to attractive spectroscopic features. The non-covalent interactions of water-soluble achiral porphyrins with biomolecules have been exploited to detect and/or stabilize different conformation adopted by DNA.[5] In this study, non-chiral porphyrins were utilized to exploit their dual capabilities: interacting with G-quadruplex structures and functioning as chiroptical probes using spectroscopic techniques, such as circular dichroism.[6] This allowed for the design of selective probes capable of distinguishing between antiparallel and parallel RNA G-quadruplexes, as well as modulating their thermodynamic stability.

REFERENCES

1. B. Pan, Y. Xiong, K. Shi, J. Deng, M. Sundaralingam, *Structure,* **2003**, 11, 815-823.
2. C. F. Tang, R. H. Shafer, *J. Am. Chem. Soc*. **2006**, 128, 5966-5973.
3. C. Xiao, T. Ishizuka, Y. Xu, *Sci. Rep.* **2017**, 7, 6695.
4. C. Xiao, T. Shibata, Y. Yamamoto, Y. Xu, *Chem. Commun*. **2018**, 54, 3944-3946.
5. a) A. D'Urso, A. G. Petrovic, M. E. Fragalà, M. A. Tamargo, G. A. Ellestad, R. Purrello, N. Berova Chapter in "DNA in Supramolecular Chemistry and Nanotechnology" **2014**, Eds. Dr Eugen Stulz and Dr Guido H. Clever, John Wiley & Sons, DOI: 10.1002/9781118696880.ch3. b) A. D'Urso, M. E. Fragalà, R. Purrello "Non-Covalent Interactions of Porphyrinoids with Duplex DNA" In: Paolesse R. (eds) Applications of Porphyrinoids. Topics in Heterocyclic Chemistry, vol 34. Springer, Berlin, Heidelberg. **2013**, cap. 5, pp 139-174. DOI: 10.1007/7081_2013_113.
6. N.C. Sabharwal, J. Chen, J. Hyun Lee, C.M.A. Gangemi, A. D'Urso, L. Yatsunik *Int. J. Mol. Sci.*, **2018**, 19, 3686-3704.

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Structure–Property Modulation in Porphyrinoids: A Molecular Roadmap from Anticancer Photodynamic Therapy to Antimicrobial Photodynamic Inactivation

Janusz M. Dąbrowski[a]

[a]*Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*

The development of light-responsive molecular systems offers exciting opportunities to address two major global challenges: drug-resistant infections and cancer. Photodynamic therapy (PDT), which relies on photosensitizer activation by light to generate reactive oxygen species (ROS), is a versatile, minimally invasive, and precisely controllable therapeutic approach applicable to both oncology [1-2] and microbiology [3].

Porphyrinoid-based photosensitizers constitute a modular molecular platform whose properties can be rationally tuned through metal ion coordination, peripheral substitution, π-system reduction, controlled asymmetry, and nanoscale formulation. Coordination with Zn(II), Pd(II), or Pt(II) allows modulation of intersystem crossing rates and singlet oxygen yields, while fluorination, sulfonamide or cationic substituents enhance solubility, cell uptake, and microbial affinity. Macrocycle reduction to bacteriochlorins extends absorption into the NIR region, enabling deep-tissue activation. Introducing molecular asymmetry and supramolecular conjugation with amino acids, antibodies, or nanoparticles further enhances selectivity, biocompatibility, and theranostic potential [4-5].

Comprehensive photophysical studies, including transient absorption spectroscopy and time-resolved singlet oxygen phosphorescence, established structure–activity relationships: long-lived triplet states and oxidation potentials correlated with balanced ROS generation and photostability. Biological validation in 2D and 3D cellular models as well as *in vivo* experiments confirmed distinct structure-dependent outcomes: compact, cationic porphyrins [3] as well as Zn(II) and Pd(II) complexes [4] exhibited superior antimicrobial activity, while amphiphilic bacteriochlorins were highly effective in NIR-driven, tumor-selective PDT [5].

These results provide a unified design framework linking electronic structure and redox properties with biological function. Effective PSs for aPDT require high photostability, efficient cellular uptake, and favorable redox profiles, whereas successful cancer PDT depends on optimized triplet lifetime, type I/II ROS balance, and stability under hypoxia. Rational structural modulation across porphyrinoid families thus enables tailoring of the same molecular scaffold for antimicrobial or oncological applications, bridging fundamental photochemistry with translational medicine.

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REFERENCES

1. P. Repetowski, M. Warszyńska, J. M. Dąbrowski, *Adv. Colloid Interface Sci.*, 2025, 336, 103356.
2. M. Warszyńska, P. Repetowski, J. M. Dąbrowski, *Coord. Chem. Rev.*, 2023, 495, 215350.
3. B. Pucelik, A. Bazowska, A. Sułek, M. Werłos, J. Dąbrowski, *Photochem. Photobiol. Sci.*, 2024, 23, 539–560.
4. M. Silva, R. Aroso, J. Dabrowski et. al., *Photochem. Photobiol. Sci*., 2024, 23, 1129-1142.
5. P. Repetowski, M. Warszyńska, J. M. Dąbrowski, *ACS Appl. Mater. Interfaces*, 2024, 16, 48937–48954.
6. M. Warszyńska, P. Repetowski, J. M. Dąbrowski, *ACS Appl. Mater. Interfaces*, 2024, 16, 50389–50406.

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Confined by Porphyrins: Molecular Cages with Exceptional Cooperative Host–Guest Interactions

Alberto de Juan[a,b], A. Priscila Gia[a], Beatriz Torres-Calvo[a], David González-Rodríguez[a,b]

[a] *Molecular Systems and Materials Group, Organic Chemistry Department, Science Faculty, Autonomous University of Madrid, Spain*
[b] *Institute for Advanced Research in Chemical Sciences (IAdChem), Autonomous University of Madrid, Spain.*

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In *Nature*, there is an omnipresent family of molecules (**porphyrinoids**) involved in most (photo)chemical events that transform solar energy into chemical energy, by consuming and regenerating O_2, H_2O, CO_2, H_2 in a closed cycle.[1] **Porphyrins** are π-conjugated macrocycles responsible for executing many of the essential life processes, such as oxygen transport/storage (*hemoglobin* and *myoglobin*), electron transfer (*cytochrome b5*), enzymatic oxidation/oxygenation (*cytochromes P450*, *peroxidases*), and converting sunlight in photosynthetic systems (*chlorophylls*).
Moreover, porphyrin reactivity and symmetry enable their functionalization in different positions, providing high versatility in self-assembly processes. Accordingly, numerous examples of porphyrin-based organic molecular cages have been reported, demonstrating their exceptional ability to host various molecules and their interesting (photo)catalytic properties.[2-3]
Here, we report the formation of two distinct porphyrin-based molecular cages constructed by linking two porphyrins via four spacers using either **dynamic imine bonds** or **hydrogen-bonding** interactions (Figure 1). These architectures provide confined, adaptable cavities, enabling in-depth study of their host–guest properties. The cages exhibit the ability to accommodate a broad range of ligands, showing in most cases a pronounced cooperative chelate effect arising from mutual host–guest conformational adaptation, reaching record *effective molarity* values above 10^3 M (Figure 1). Furthermore, the host's relatively high rigidity enables the *selective* encapsulation of guest molecules of varying sizes.[4]

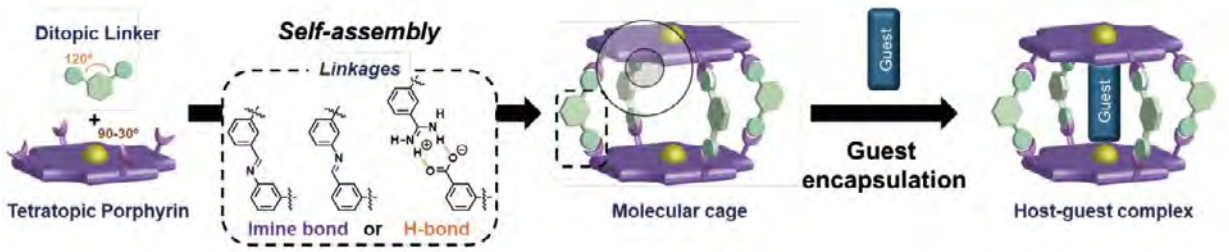


Figure 1. Schematic representation of molecular cage self-assembly and host-guest complex formation.

REFERENCES

1. IPCC Climate Change. The physical science basis. **2013**, *1535*.
2. R. Guilard, K. M. Kadish, K. M. Smith, *The porphyrin handbook*. Academic Press New York: **2003**; Vol. 18.
3. S. Durot, J. Taesch, V. Heitz, *Chem. Rev*. **2014**, *114*, (17), 8542.
4. A. P. Gia, A. de Juan, D. Aranda, F. G. Guijarro, J. Aragó, E. Ortí, M. García-Iglesias, D. González-Rodríguez, *J. Am. Chem. Soc.* **2025**, *147*, 918.

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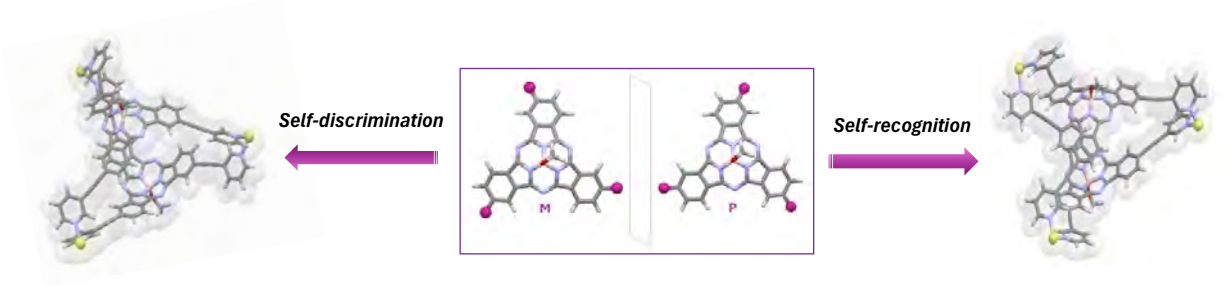
Chiral Self-Sorting in Subphthalocyanine-Based Metallosupramolecular Cages

Gema de la Torre[a,b], **Ainhoa Salazar**[a], **David Sánchez-Fernández**[a], **Patricia Calvo**[a]

[a] *Organic Chemistry Department, Universidad Autónoma de Madrid, 28049 Madrid, Spain.*
[b] *Institute for Advanced Research in Chemical Sciences, Universidad Autónoma de Madrid, 28049 Madrid, Spain*

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The design of metallo-organic cages that mimic enzymatic cavities has emerged as a powerful strategy for promoting and controlling chemical transformations [1]. Metallosupramolecular subphthalocyanine-based cages ($SubPc_2Pd_3$), constructed from a C_3-symmetric SubPc functionalized with three pyridyl donor ligands and Pd(II)-diamine complexes, have shown to function as catalytic molecular containers capable of accelerating addition reactions overfullerenes [2]. In particular, a water-soluble $SubPc_2Pd_3$ cage performs as a hydrophobic nanoreactor for Diels–Alder cycloadditions with encapsulated C_{60} and C_{70} [3,4]. This nanocontainer overcomes limitations such as product inhibition, enabling catalysis in aqueous media. All these results have been achieved with heterochiral $SubPc_2Pd_3$ cages, wich are a result of the predominant self-discrimination process of the racemic mixture of M and P ennationer present in the C_3-symmetric tris-functionalized SubPcs as a consequence of their bowl-shape structure and configurational stability.
In this presentation, we describe the results on tuning the chiral self-assembly of these systems. The interplay between different Pd(II) salts, diamine ligands, and counterions governs the narcissistic (homochiral) versus social (heterochiral) sorting processes, leading to assemblies with distinct chiral configurations. Moreover, interconversion of these chiral architectures via anion exchange have been examined, revealing new avenues for dynamic control over cage chirality, and chiral recognition abilities of certain guests.



REFERENCES

1. Pujals. M; Pèlachs. T; Fuertes-Espinosa. C; Parella. T; Garcia- Borrà, M; Ribas. X. *Cell Rep. Phys. Sci*. **2022**, *3*, 100992.
2. Moreno-Simoni, M; de la Torre, G; Torres, T. *Chem. Sci.* **2022**, *13*, 9249.
3. Salazar. A; Moreno-Simoni. M; Kumar. S; Labella. J; Torres. T; de la Torre. G. *Angew. Chem. Int. Ed*. **2023**, *62,* e202311255.
4. Salazar. A; Kumar. S; Labella. J; Torres. T; de la Torre. G. *Adv. Synth.Catal.* **2024**, *366*, 934.

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On-surface Synthesis of Porphyrin-Based MONs: a Model System for Catalysis and Artificial Spin Lattices

Abner de Siervo[a]

[a]*Institute of Physics Gleb Wataghin, University of Campinas (UNICAMP), 13083-859 Campinas, Brazil*

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Over the past decade, significant advances have been achieved in the on-surface synthesis of atomically precise one-dimensional (1D) and two-dimensional (2D) metal–organic networks (MONs) using selected molecular precursors as modular building blocks in a "molecular LEGO" approach. This strategy exploits substrate properties, precursor molecular geometry and functional groups, as well as diffusion behavior and thermal activation energies, to steer hierarchical reactions and the formation of novel nanostructures [1]. Porphyrins and phthalocyanines, owing to their well-defined geometry and rich electronic properties, have emerged as particularly promising building blocks. Their chemical versatility enables the design of functionalized derivatives that enhance on-surface reactions and polymerization processes. When their molecular periphery is terminated with cyano, pyridyl, or halogen groups, deposited or substrate-derived adatoms can be trapped to form metal–organic coordination nodes. This leads to MONs with linear, square, rectangular, hexagonal, or kagome lattices, with geometries dictated by the molecular structure and substrate registry. Such architectures serve as important model systems for gaining deeper insight into the physical and chemical mechanisms underlying host–guest chemistry, photocatalysis, and two-dimensional artificial spin lattices, among other phenomena. In this seminar, I will present recent examples of MON formation using two types of free-base porphyrins: 5,10,15,20-tetrakis(4-bromophenyl)porphyrin (H_2TBrPP) [2] and 5,10,15,20-tetra(4-pyridyl)porphyrin (H_2TPyP), adsorbed on Ag(100) surfaces [3]. For H_2TBrPP on Ag(100), we demonstrate the formation of both 1D and 2D MONs, characterized by distinct molecular conformations—an inverted geometry in the 1D chain case and a saddle-shape conformation in the 2D network [2]. In contrast, H_2TPyP on Ag(100) yields 2D MONs as well as extended, ordered spin lattices when Fe adatoms are introduced during on-surface synthesis. These different structures can be selectively realized by controlling the annealing protocol and the sequence of Fe deposition [3,4]. These studies combine scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) experiments, supported by density functional theory (DFT) calculations.

REFERENCES

1. J. Barth, G. Costantini, K. Kern, *Nature* **437,** 671–679 (2005).
2. Nataly Herrera-Reinoza et al., The Journal of Physical Chemistry C 129 (19), 9085-9096 (2025).
3. Rafael Reis Barreto, et al., Surface Science 766, 122897 (2026).
4. Rafael Reis Barreto, et al., "Engineering Two-Dimensional Artificial Spin Lattice Based on Porphyrins Metal-Organic Networks" (under preparation).

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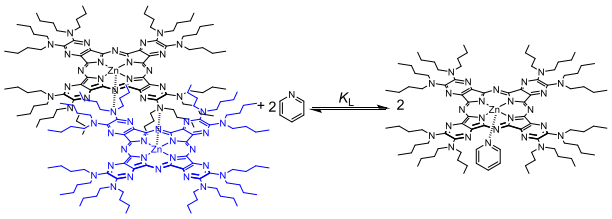
J-dimers of Tetrapyrazinoporphyrazines

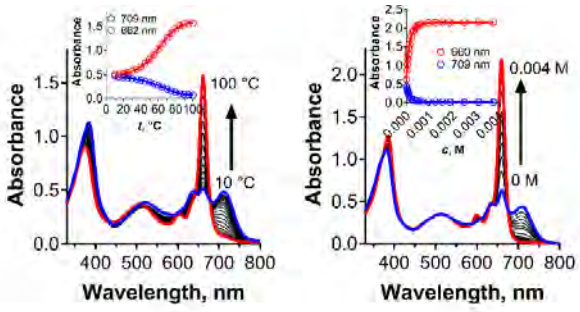
J. Demuth,[a] R. Machan,[a] I. Mocak,[a] T. Malinsky,[a] M. A. El Dahabova,[a] J. Holcak,[a] S. Bednarik,[a] M. Miletin,[a] J. Labuta,[b] V. Novakova,[a] P. Zimcik[a]

[a]Faculty of Pharmacy in Hradec Králové, Charles University, Akademika Heyrovskeho 1203/8, 500 05 Hradec Kralove, Czech Republic;
[b]Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

Tetrapyrazinoporphyrazines (TPyzPzs) are planar macrocyclic compounds with spectacular photophysical properties due to their large aromatic system. TPyzPzs bearing dialkylamino substitution on the periphery can form supramolecular assemblies called J-dimers in non-coordinating solvents, due to the interaction of the peripheral amine of compound one with the central metal cation of the second compound (left figure).[1] Formation of J-dimer influences photophysical properties of TPyzPzs (spectra, production of singlet oxygen and fluorescence) (right figure). For the dissolution of aggregates, ligands with higher binding ability to the central metal cation than the coordination moiety are necessary[2]

In the first part of this study, symmetrical TPyzPzs with different bulkiness of peripheral dialkylamine substitution were synthesized. These compounds were studied from an aggregation perspective. Results led us to the synthesis of unsymmetrical TPyzPz derivatives composed of 3 bulky precursors and 1 small one. The final step was switching from non-fluorescent oktakis(dialkylamino) TPyzPzs to alkylsulfanyl to compare the influence of electron effects of peripheral substitution on the stability of J-dimers.





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REFERENCES

[1] V. Novakova et al., Eur. J. Org. Chem., 2008, (19), 3260-3263.)
[2] J. Demuth et al., Inorg. Chem. Front., 2025,12, 1590-1608

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Radiation-activated photodynamic therapy for rectal cancer treatment

Wei Deng[a], Rui Sang[b], Tzongtyng Hung[c], Alexander Engel[d], Ewa M. Goldys[b]

[a]*The School of Biomedical Engineering, Faculty of Engineering and IT, University of Technology Sydney, Broadway, NSW, Australia*
[b]*The School of Biomedical Engineering, University of New South Wales, Kensington, NSW, Australia*
[c]*Biological Resources Imaging Laboratory, UNSW Sydney, Sydney, NSW, 2052, Australia*
[d]*Sydney Medical School, University of Sydney, Sydney, NSW, Australia*

Rectal cancer accounts for approximately 30% of colorectal cancers, which is the 2nd most deadly cancer in Australia [1]. A significant proportion of Stage III rectal cancer patients undergo chemo-radiotherapy to downsize the primary tumour and lymph node metastasis before surgery [2]. Unfortunately, the side effect of this standard of care treatment is progressive late morbidity due to high doses in long-course radiotherapy and toxicity of chemotherapeutic drugs used in chemo-radiotherapy [3]. To improve the quality of life of rectal cancer patients, it is important to find a new and safe treatment method. Here, we brought a new treatment method, radiation-activated photodynamic therapy (RA-PDT), by combining existing clinical techniques used in cancer treatment and delivering via bespoke nanocarriers. In this strategy, verteporfin (VP), a clinically approved photosensitizer, was directly activated by radiation via a lipid-polymer hybrid nanoplatform. The activated VP generates highly toxic reactive oxygen species, killing the cancer cells. With X-PDT, the tumour growth suppression was observed in an orthotopic mouse model bearing rectal cancer. Such tumour control is consistent with decreased cell viability, increased necrotic tumour tissue, and reduced Ki-67 protein expression observed in the mouse group treated with RA-PDT, compared with other treatment conditions. Our study establishes an effective strategy to treat rectal cancer in a more clinically relevant model, which offers prospects for clinical translation of this technology for deep-seated cancers.

REFERENCES

1. Morgan E, Arnold M, Gini A, et al. Global burden of colorectal cancer in 2020 and 2040: incidence and mortality estimates from GLOBOCAN. Gut. 2023;72:338–344.
2. Kim TH, Jeong SY, Choi DH, et al. Lateral lymph node metastasis is a major cause of locoregional recurrence in rectal cancer treated with preoperative chemoradiotherapy and curative resection. Ann Surg Oncol. 2008;15:729–737.
3. Feeney G, Sehgal R, Sheehan M, et al. Neoadjuvant radiotherapy for rectal cancer management. World J Gastroenterol. 2019;25(33): 4850–4869.

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Defining heme pocket factors that drive ligand selectivity in the carbon monoxide sensor protein *Px*RcoM-1

Matthew R. Dent[a], Nisa R. Mahmood[a], Mustafa K. Alithawi[a], Jayani Nissanka[a]

[a]*Department of Chemistry, Wayne State University, Detroit, MI, USA*

ORALS

Carbon monoxide (CO) is both a lethal environmental toxin and a biologically active signaling molecule with emerging therapeutic potential.[1] Generated by nearly all organisms on Earth as an enzymatic by-product of heme breakdown, CO influences cellular processes including inflammation, cell proliferation, and apoptosis.[2-4] CO binds tightly to ferrous heme iron, and this metal-ligand binding has largely shaped our understanding of CO as a poison and signal. While this coordination chemistry is well understood, specific protein targets that mediate CO-dependent signal transduction remain elusive. A key knowledge gap is the lack of unifying principles that identify a heme pocket as selective for CO over other biological gases like oxygen, nitric oxide, and hydrogen sulfide. To bridge this gap, we have quantified ligand binding parameters in the microbial CO-sensing transcription factor *Px*RcoM-1 (regulator of CO metabolism 1 from the soil aerobe *Paraburkholderia xenovorans*). *Px*RcoM-1 is a CO-dependent, single-component transcriptional activator of the *cox* operon, which encodes an oxygen-tolerant, Cu,Mo-dependent CO dehydrogenase.[5,6] Remarkably, RcoM utilizes a heme cofactor to sense trace atmospheric levels of CO (~100 ppb) in an aerobic background, suggesting extreme preference for CO binding over O_2. Consistent with this functional role, we found that *Px*RcoM-1 exhibits high CO affinity ($K_{d,CO}$ = 16 nM) but no quantifiable binding to O_2. We hypothesized that unique CO selectivity of RcoM is driven by the structure of the distal heme pocket, which contains highly conserved bulky hydrophobic and aromatic amino acid residues that may restrict diatomic ligands to bind in a linear fashion. To test this hypothesis, we have generated RcoM variants bearing alterations to conserved distal pocket residues that change steric bulk, hydrophobicity, and presence of charged groups and H-bond donors. We observe significant changes in CO and O_2 binding affinities, heme redox properties, and ligand-dependent DNA binding of distal pocket variants, and the functional implications of these changes will be discussed.

REFERENCES

1. Bansal, S. et al. *J. Med. Chem.* **2024**, *67* (12), 9789–9815
2. Yuan, Z. et al. *Pharmacol. Rev.* **2022**, *74* (3), 823–873.
3. Kim, H. J. et al. *Cell Death Dis.* **2018**, *9* (11), 1060.
4. Otterbein, L. E. et. al. *Circ. Res.* **2016**, *118* (12), 1940–1959.
5. Kerby, R. L. et al. *J. Bacteriol.* **2008**, *190* (9), 3336–3343.
6. Dent, M. R. et al. *Biochemistry* **2022**, *61* (8), 678–688.

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Design and evaluation of the antimicrobial activity of new corroles and porphyrins functionalized with carboxylic or phosphonic acids

Nicolas Desbois,[a] Gaëlle Divoux,[a] Matthias Roux,[a] Marc Sautour,[b,c] Stéphane Brandès,[a] Claude P. Gros[a]

[a]*Université Bourgogne Europe, ICMUB UMR CNRS 6302, 21000 Dijon, France*
[b]*Parasitology-Mycology Laboratory, University Hospital Biology Platform, Dijon University Hospital Center (CHU), 21000 Dijon, France*
[c]*Université Bourgogne Europe, Institut Agro, INRAE, UMR PAM, 21000 Dijon, France*

Antibiotics are commonly used to treat, prevent, or control bacterial infections. However, microorganisms have developed several resistance mechanisms to standard treatments. Bacterial resistance has therefore increased considerably in recent years, particularly in hospital settings, rendering some therapies ineffective. Regarding antifungal compounds, resistance to azoles is a major obstacle to clinical success. To mitigate this emerging public health problem, it is necessary to develop new antimicrobial techniques that are non-invasive, non-toxic, and more effective and rapid than current antimicrobial molecules. We recently demonstrated that corroles and porphyrins functionalized with two carboxylic acid groups exhibit very promising antimicrobial activity, with or without PDI (photodynamic inactivation) [1-2]. We will present our progress, including the replacement of carboxylic acid groups with phosphonic acid groups. We will also explore the integration of these new photosensitizers into metal-organic structures (MOFs). We aim to obtain new products with enhanced antimicrobial activity.

REFERENCES

1. M. Sautour, S. Pacquelet, C. P. Gros, N. Desbois, *Bioorg. Med. Chem. Lett.,* **2023**, 82, 129167.
2. M. Sautour, T. Théry, S. Dupont, L. Beney, C. P. Gros, N. Desbois, *Bioorg. Med. Chem.* **2024**, 109, 117810.

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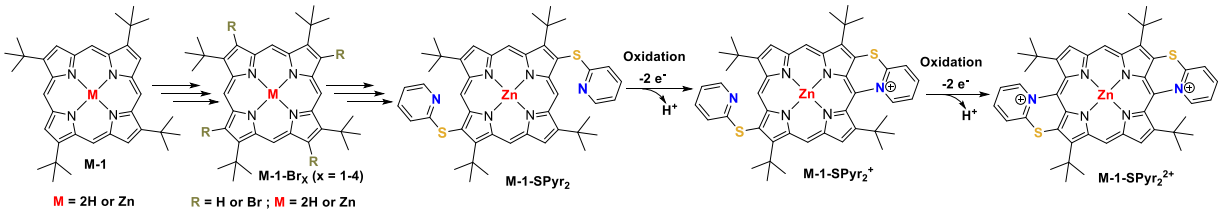


Unusual *β*-Bromination of the *meso*-Free 2,7,12,17-Tetra-*tert*-butylporphyrin. Thiopyridinyl Functionalization of the bis-*β*-Brominated porphyrin for the synthesis of C_{meso}-N Fused Porphyrins

Nesrine Amiri[a], Amelle Mankou-Makaya[a], Hélène Cattey[a], Charles H. Devillers[a]

[a] *Université Bourgogne Europe, CNRS, Institut de Chimie Moléculaire de l'Université de Bourgogne (ICMUB, UMR CNRS 6302), 9 avenue Alain Savary, 21078 Dijon Cedex, France*

Porphyrins are versatile π-conjugated macrocycles which have found among others, applications in catalysis,[1] sensing,[2] photovoltaics,[3] and photodynamic therapy.[4] Chemical modifications at the *β*-pyrrolic positions are of particular interest, as they strongly influence the structural and electronic properties of the porphyrin core. In this work, we report the synthesis of a new series of *β*-brominated 2,7,12,17-tetra-*tert*-butylporphyrins and their zinc(II) complexes, using *N*-bromosuccinimide as the brominating agent. By controlling the reaction conditions, mono-, di-, tri- and tetra-brominated derivatives were isolated in moderate to excellent yields (Scheme 1, left). The compounds were fully characterized by NMR spectroscopy, mass spectrometry, UV–Vis absorption spectroscopy, and for some of them, by X-ray diffraction analysis. Then, the bis-brominated porphyrin **M-1-Br$_2$** was functionalized with two thiopyridinyl moieties to afford Zn(II) *β*-pyridin-2-ylthio-porphyrin **M-1-Spyr$_2$** (Scheme 1, middle). Electrochemical oxidation of **M-1-Spyr$_2$** led to intramolecular C–N bond formation, giving mono- (**M-1-Spyr$_2^+$**) and bis-fused (**M-1-Spyr$_2^{2+}$**) macrocycles. These fused derivatives exhibit important change in their electronic properties due to enhanced conjugation.



Scheme 1: *β*-bromination of **M-1** and C_{meso}-N oxidative fusion of **M-1-SPyr$_2$**.

REFERENCES

1. Li, X.; Lei, H.; Xie, L.; Wang, N.; Zhang, W.; Cao, R. Metalloporphyrins as Catalytic Models for Studying Hydrogen and Oxygen Evolution and Oxygen Reduction Reactions. *Acc. Chem. Res.* **2022**, *55* (6), 878–892. https://doi.org/10.1021/acs.accounts.1c00753.
2. Di Zazzo, L.; Kumar, A.; Meunier-Prest, R.; Di Natale, C.; Paolesse, R.; Bouvet, M. Electrosynthesized Copper Polycorroles as Versatile Materials in Double Lateral Heterojunctions. *Chem. Eng. J.* **2023**, *458*, 141465. https://doi.org/10.1016/j.cej.2023.141465.
3. Huang, S.; Li, Q.; Li, S.; Li, C.; Tan, H.; Xie, Y. Recent Advances in the Approaches for Improving the Photovoltaic Performance of Porphyrin-Based DSSCs. *Chem. Commun.* **2024**, *60* (34), 4521–4536. https://doi.org/10.1039/D3CC06299F.
4. Ethirajan, M.; Chen, Y.; Joshi, P.; Pandey, R. K. The Role of Porphyrin Chemistry in Tumor Imaging and Photodynamic Therapy. *Chem. Soc. Rev.* **2011**, *40* (1), 340–362. https://doi.org/10.1039/B915149B.

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Porphyrin-conductive polymer hybrids for high sensitive and selective detection of volatile compounds

Rosamaria Capuano[a,b], Valerio Allegra[a], Alexandro Catini[a,b], Gabriele Magna[b,c], Roberto Paolesse[b,c], Corrado Di Natale[a,b]

[a]*Department of Electronic Engineering, Tor Vergata University of Rome, Rome, Italy*
[b]*Interdepartmental. Centre for Volatilomics "A.D'Amico", Tor Vergata University of Rome, Rome, Italy*
[c]*Department of Chemical Sciences and Technology, Tor Vergata University of Rome, Rome, Italy*

Porphyrinoids are distinguished by their capability to exploit rich molecular motifs for binding airborne compounds [1]. The structure of porphyrinoids comprises two primary components: peripheral substituents and a central metal ion, each contributing to the molecule's overall selectivity. Additionally, modifications of the macrocyclic skeleton give rise to porphyrin analogues with distinct properties [2].
Despite their extensive aromatic systems, solid aggregates of porphyrinoids are typically nonconductive. Therefore, convenient methods for preparing resistive sensors involve coupling porphyrinoids with organic or inorganic semiconductors. Among the available combinations, we have explored hybrids of porphyrinoids and wide-bandgap semiconductors, capitalizing on the possibility of combining sensitivity to both light and chemicals for the development of self-powered devices [3].
An alternative approach considers blends of conductive polymers and porphyrins. Recently, we developed an array composed of different blends of porphyrins and poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), a p-type conductive polymer widely used in organic electronics and chemical sensing.
Doping PEDOT:PSS with metal ions has been shown to enhance the sensitivity of gas sensors, particularly toward electron-donor molecules. On this basis, we investigated the sensitivity of porphyrin–PEDOT:PSS blends and observed a strong response to ammonia. Residual sensitivity to other volatile organic compounds (VOCs) enables the identification of species present at higher concentrations. This property was exploited to develop a disposable sensor array on a flexible substrate embedded in facemasks for breath analysis. The sensors were successfully applied to the diagnosis and prognosis of chronic kidney disease [4].
The simplicity of fabrication, combined with recent advances in additive manufacturing technologies, enables the scalable production of low-cost, high-performance sensor platforms. These features position porphyrin-based hybrid devices as promising candidates for next-generation wearable and disposable sensing systems, with significant potential for real-time chemical monitoring and non-invasive medical diagnostics.

REFERENCES

1. Paolesse, R.; Nardis, S.; Monti, D.; Stefanelli, M.; Di Natale, C. *Chem. Rev.* **2017**, 117, 2517−2583
2. Di Natale, C., Gros, C., Paolesse, R., *Chem Soc Rev*, **2022**, 51, 1277-1355
3. George, J., Vikraman, H., Ghuge, R., Reji, R., Jayaraman, S, Magna, G., Paolesse, R.,Sivalingam, Y.,Di Natale, C., Mangalampalli, K., *Small*, **2025**, 2502324
4. Capuano, R., Allegra, V., Catini, A., Magna, G., Di Lauro, M., Marrone, G., Agresti, A., Pescetelli, S., Pieri, M., Paolesse, R., Bernardini, S., Noce, A., Di Natale, C. *ACS Sens,* **2025**, 10 , 4850-4861

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Protein-Mediated Export of Coproporphyrin III and its Role in Maintaining Heme Homeostasis in Mycobacteria

Rebecca K. Donegan[a], Grace Wang[a], Jessica Samudio[a], Hadia Aftab[a], Lily Le[a], and Fereshteh Zandakrimi[b,c]

[a]*Department of Chemistry, Barnard College, Columbia University, New York, NY 10027*
[b]*Department of Chemistry, Columbia University, New York, NY, USA*
[c]*Mass Spectrometry Core Facility, Columbia University, New York, NY, USA*

Many Gram-positive bacteria, including the nontuberculous mycobacteria, secrete coproporphyrin III (copro) for various outcomes. However, unlike in the classical protoporphyrin-dependent pathway, copro is not an off-pathway waste product but a heme biosynthesis intermediate.[1] In our attempt to understand how copro secretion may alter heme homeostasis in these organisms, we have found that intracellular heme levels are effectively decoupled from copro flux, as the addition of porphyrin precursors does not alter internal heme levels.[2] We have also found that the addition of the extracellular porphyrin-binding protein albumin increases porphyrin export and that Msm secretes proteins that copurify with copro [2]. Collectively, our results indicate that porphyrin export is a protein-mediated, regulated process rather than a metabolic leak, possibly serving a biological role in the mycobacterial life cycle.

REFERENCES

1. Dailey, Harry A., et al. "Prokaryotic heme biosynthesis: multiple pathways to a common essential product." *Microbiology and Molecular Biology Reviews* 81.1 (2017): 10-1128.
2. Wang, Grace, et al. "Porphyrin secretion does not alter heme biosynthesis in the nontuberculous mycobacteria." Journal of Inorganic Biochemistry (2025): 113151.

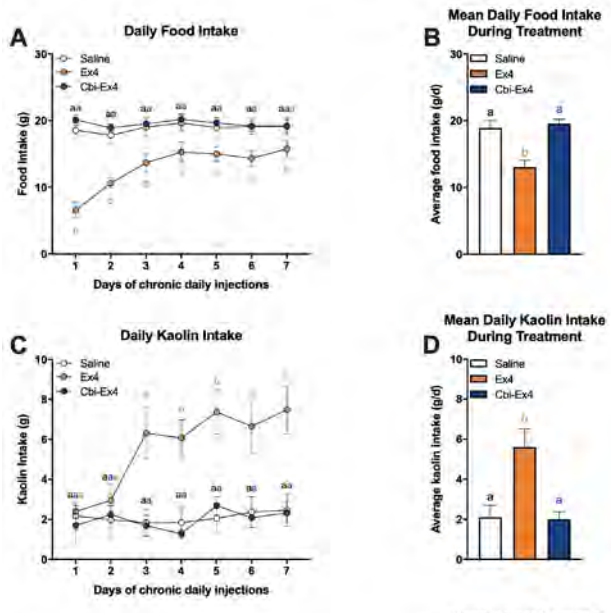
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Dicyanocobinamide conjugates of Exendin-4 confers glucoregulation without weight-loss or nausea in tumour-bearing rats

Robert P. Doyle[a], Nancy Cham,[b] Bart C. De Jonghe[b], Matthew R. Hayes[b], Tito Borner[C]

[a]*Syracuse University, Syracuse, NY 13244, USA*
[b]*University of Pennsylvania, Philadelphia, PA, USA*
[c]*University of Southern California, Los Angeles, CA, USA*

Recently, the term "corrination" was coined to describe the conjugate modification of a peptide, protein, small molecule, or radionuclide with a corrin ring-containing molecule [1]. By exploiting the innate chemicophysical properties of corrin ring-containing compounds, corrination has been explored for drug development and targeted/localized delivery of probes and therapeutics. Peptide-based drugs possess several limitations that restrict their clinical application, including negative side effects often due to drug distribution. Despite being a common medication for the treatment of Type 2 Diabetes (T2D), activation of the GLP-1 receptor (GLP-1R) in the brain by peptide-based GLP-1R agonists results in weight loss and gastrointestinal (GI) side effects, such as nausea and emesis [2-3]. These side effects are a significant reason for the discontinuation of this medication among patients with T2DM, and due to the resulting weight loss, certain subpopulations with comorbidities where nutritional status is critical, such as those with cancer, cannot use GLP-1R analogs. Therefore, there is a clinical need for effective GLP-1-based analogs that circumvent weight-loss and GI side effects in cancer patients with co-morbid T2DM. Herein, we show that a corrinated GLP-1R agonist confers glucoregulation without weight loss and is devoid of nausea in tumour-bearing rats.



REFERENCES

1. Corrin Ring Modification in Peptide Drug Development–a Brief History of "Corrination". N Cham, RP Doyle. *ChemMedChem* 20 (10), e202500129, **2025**.
2. Glucagon-like peptide-1 in diabetes care: Can glycaemic control be achieved without nausea and vomiting?. T Borner, IC Tinsley, RP Doyle, MR Hayes, BC De Jonghe. *British Journal of Pharmacology* 179 (4), 542-556, **2022.**
3. Synthesis, optimization, and biological evaluation of corrinated conjugates of the GLP-1R agonist exendin-4. IC Tinsley, T Borner, MKL Swanson, OG Chepurny, SA Doebley, V Kamat, RP Doyle. *Journal of Medicinal Chemistry* 64 (6), 3479-3492, **2021**.

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Hetero-Annelated Porphyrazines and Subporphyrazines: Promising Photosensitizers and Luminophores

Tatiana V. Dubinina[a], Mikhail S. Belousov[a], Roman O. Eremeev[a], Mikhail R. Antanyazov[a], Maria M. Ivanova[a], Ivan D. Burtsev[b], Alina A. Markova[b], Vladimir A. Kuzmin[b]

[a]*Moscow State University, 1 Leninskie Gory, 119991 Moscow, Russia*
[b] *Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Kosygin st., 4, 119334 Moscow, Russia*

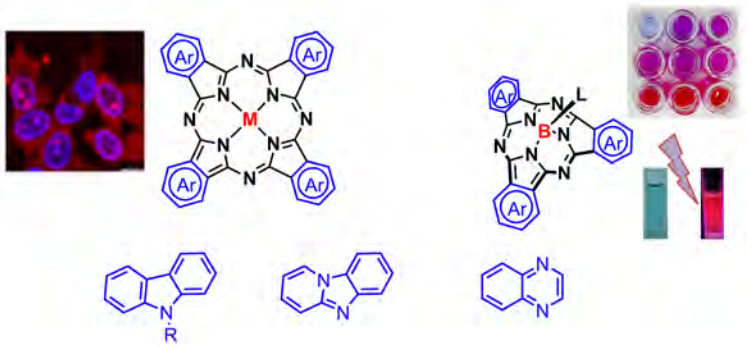
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A series of π-extended porphyrazines and boron subporphyrazines with absorption in the high transparency region of biological tissues (600-800 nm) were obtained. Pyrido[1,2-a]benzimidazole, carbazole, and quinoxaline heterocycles were chosen for the annulation of the tripyrrolic and tetrapyrrolic cores for the following reasons: (1) Pyrido[1,2-a]benzimidazoles can be quaternized to give water-soluble porphyrazines; (2) Various functional groups can be attached to the carbazole nitrogen atom; and (3) The electron-deficient quinoxaline heterocycle can enhance the oxidative stability of the macrocycle.

Novel pyrido[1,2-a]benzimidazole-fused tetrapyrrolic photosensitizers with an intense near-infrared absorption (711–747 nm) were prepared. Water-soluble quaternized forms of target photosensitizers demonstrated low cytotoxicity in the dark and submicromolar photodynamic activity against A549, WI38, HCT116, MCF7, A431 and HeLa cell lines. Their photodynamic index value is approximately 2 times higher than that of chlorin e6, a well-known component of photosensitizers approved for photodynamic therapy, such as *Photolon*, *Photoditazine*.

Carbazole-fused porphyrazines and their solubilized forms exhibiting photocytotoxicity (up to IC_{50} = 0.33 μM) were obtained. Synthetic approaches to carbazole-fused boron subporphyrazines were developed and it was shown that they are both effective photosensitizers (Φ_{Δ}=0.42) and bright fluorophores (Φ_f=0.24).

New classes of quinoxaline-fused boron subporphyrazines and the stability of their solutions in various organic solvents were demonstrated. By-products of electrophilic chlorination of quinoxaline fragments formed during template synthesis were isolated. Conditions for completely suppressing the chlorination process were found. We also studied the influence of the solvent type on the spectral properties and stability of the new compounds and compared these data with similar experiments with the described subphthalocyanines and subporphyrazines [1].



The work was supported by Russian Science Foundation, grant number 23-73-10076.

REFERENCES

1.Eremeev R.O. et al. // Dyes and Pigments 241 (2025) 112868.

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A Widespread System for Anaerobically Removing Iron from Heme

Jennifer L. DuBois, Emmanuel Akpoto, Sal Martoglio, Arnab Kumar Nath, Ronivaldo Rodrigues da Silva

Department of Chemistry and Biochemistry, Montana State University

Biological heme degradation under aerobic conditions, in which O_2 is used to oxidatively cleave the conjugated porphyrin ring, is well understood. However, heme is catabolized by microbiota for its iron under anaerobic conditions, including inside the gastrointestinal tract (GI), anoxic wounds, compost heaps, and bioreactors. We describe a broadly conserved mechanism for removing iron from heme, leaving behind protoporphyrin IX. The HmuS enzyme acts as a de-chelatase in conjunction with other proteins that may serve to deliver heme or retrieve the porphyrin. This reaction may play a critical role in the digestion of heme by abundant Bacteroidetes species in the GI tract microbiome, and in the generation of porphyrins by pathogenic strains in anoxic wounds.

REFERENCES

1. Kumar Nath A, da Silva RR, Gauvin CC, Akpoto E, Dlakić M, Lawrence CM, DuBois JL. Commensal gut bacteria employ de-chelatase HmuS to harvest iron from heme. EMBO J. 2025 Nov;44(21):6226-6252. doi: 10.1038/s44318-025-00563-5.
2. Rodrigues da Silva R, Larson J, Bothner B, DuBois JL. Heme and iron limitation in a GI-tract foundation species leads to a reshuffling of the metalloproteome and a shift toward manganese usage. Front Chem. 2025 Apr 2;13:1562189. doi: 10.3389/fchem.2025.
3. Meslé MM, Gray CR, Dlakić M, DuBois JL. Bacteroides thetaiotaomicron, a Model Gastrointestinal Tract Species, Prefers Heme as an Iron Source, Yields Protoporphyrin IX as a Product, and Acts as a Heme Reservoir. Microbiol Spectr. 2023 Mar 2;11(2):e0481522. doi: 10.1128/spectrum.04815-22.
4. Coe GL, Pinkham NV, Celis AI, Johnson C, DuBois JL, Walk ST. Dynamic Gut Microbiome Changes in Response to Low-Iron Challenge. Appl Environ Microbiol. 2021 Jan 15;87(3):e02307-20. doi: 10.1128/AEM.02307-20.

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Phthalocyanines with improved properties for photodynamic applications

Fabienne Dumoulin[a,b]

[a]*Acıbadem Mehmet Ali Aydınlar University, Faculty of Engineering and Natural Sciences, Biomedical Engineering Department, 34752 Ataşehir, Istanbul, Türkiye*
[b]*Acibadem Mehmet Ali Aydinlar University, Graduate School of Natural and Applied Sciences, Ataşehir, 34752 Istanbul, Türkiye. E-mail: Fabienne.Dumoulin@acibadem.edu.tr / dumoulin.fabienne@gmail.com*

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Photodynamic applications rely on photosensitizers with high triplet quantum yields. Other specific properties are desired depending on the targeted application. Photodynamic therapy can be improved by better generation of singlet oxygen and other reactive oxygen species, often promoted by heavy atoms, and by specific tumor accumulation, both of which can be improved by drug delivery systems. On the other hand, azobenzene triplet photoswitching needs systems shielded from oxygen.

Our recent work in these areas will be presented [1-6].

REFERENCES

[1] Pui-Chi Lo, M. Salomé Rodriguez-Morgade, Dennis K. P. Ng*, Tomas Torres*, Ravindra Pandey* and Fabienne Dumoulin*, Chemical Society Reviews, 2020, 49, 1041-1056
[2] Lukas Naimovičius, Mila Miroshnichenko, Ekin Opar, Helen Hölzel, Masa-aki Morikawa, Nobuo Kimizuka, Manvydas Dapkevičius, Justas Lekavičius, Edvinas Radiunas, Karolis Kazlauskas, Víctor Cilleros-Mañé, Fabio Riefolo, Carlo Matera, Kevser Harmandar, Masahiko Taniguchi, Fabienne Dumoulin, Jonathan S. Lindsey, Pankaj Bharmoria, Pau Gorostiza, Kasper Moth-Poulsen, Nature Commun., 2025, 16, 6377.
[3] Davide Arena, Umit Isci, Mélanie Onofre, Christophe Nguyen, Zeynel Sahin, Ester Verde-Sesto, Amaia Iturrospe, Arantxa Arbe, Magali Gary-Bobo, José A. Pomposo, and Fabienne Dumoulin, Topology effects in photodynamic therapy with phthalocyanine nanocarriers, Mater. Adv. 2025, 6, 148-156
[4] Paweł Repetowski, Marta Warszyńska, Anna Kostecka, Barbara Pucelik, Agata Barzowska, Atefeh Emami, Ümit İşci, Fabienne Dumoulin* and Janusz M. Dąbrowski*, Synthesis, Photo-Characterizations, and Pre-Clinical Studies on Advanced Cellular and Animal Models of Zinc(II) and Platinum(II) Sulfonyl-Substituted Phthalocyanines for Enhanced Vascular-Targeted Photodynamic Therapy, ACS Applied Materials & Interfaces, 2024, 16, 48937−48954
[5] Zeynel Şahin, Emel Önal, Lamiaa M. A. Ali, Denis Durand, Atefeh Emami, Marie Touré, Umit Işci, Magali Gary-Bobo, Sandrine Cammas-Marion, and Fabienne Dumoulin, Nanoencapsulation of a Far-Red Absorbing Phthalocyanine into Poly(benzylmalate) Biopolymers and Modulation of Their Photodynamic Efficiency, Biomacromolecules 2024, 25, 3261−3270
[6] Aymen Nabeel Yaseen, Atefeh Emami, Haifa Ben Aziza, Merve Dandan Doganci, Ümit İşci, Ayşe Gül Gürek, Erdinc Doganci and Fabienne Dumoulin, Near infrared-absorbing self-encapsulated phthalocyanine-cored polycaprolactone star polymeric nanoparticles, J. Porphyrins Phthalocyanines 2024; 28: 107–113

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Coordinative self-assembly of π-electron magnetic porphyrins

David Écija

IMDEA Nanociencia, Madrid, Spain.

π-Electron magnetic compounds on surfaces have emerged as a powerful platform for probing spin interactions at the atomic scale. In particular, on-surface synthesis has become a powerful method for fabricating open-shell, carbon-based materials whose magnetic interactions, mediated by covalent bonding, have been systematically explored in recent years [1]. On the other hand, coordination chemistry on surfaces has been shown to promote long-range ordering by forming metal-organic frameworks. However, understanding its potential to mediate spin exchange interactions in carbon-based open-shell systems remains in its early stages.

In this work, we contribute to this field by synthesizing π-extended 3d-metal porphyrins functionalized with carbonitrile groups [2]. Our scanning probe microscopy studies show that depositing the precursor on a Au(111) surface under varying conditions leads to the formation of one-dimensional coordinative structures—either wires or nanotapes—composed of π-extended porphyrin units. Using STM tip manipulation, we selectively remove passivating hydrogen atoms from the molecules, thereby exposing their open-shell characteristics. We then study their interactions within the coordinative nanoarchitectures and with the 3D metals in the porphyrin cores. These features are analyzed through Scanning Tunneling Spectroscopy (STS) in combination with DFT and CASCI simulations. Overall, our study highlights the combined power of on-surface covalent synthesis and coordination chemistry in constructing unprecedented open-shell, low-dimensional coordination polymers, while preserving the magnetic individuality of the constituent monomers.

REFERENCES

[1] X. Li et al., Chinese Chem. Letters, 36 (2025); Q. Sun et al., Adv. Science, 9 (2022)
[2] M. Tenorio et al., Angew. Chem. Int. Ed., 64 (2025).

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The windmill, the dragon and the frog: isomerically pure α-aryl-substituted phthalocyanines, their spectral features and functions

Alexander Efimov[a], Nagao Kobayashi[b], Atsuya Muranaka[c], Aleksandr Penni[a], Viacheslav Golovanov[d], Riikka Rimmistö[e], Sebastian Pätsch[a], Nikita Durandin[a]

[a]*Tampere University, Chemistry and Advanced Materials, Korkekouluntkatu 8, 33720 Tampere, Finland*
[b] *Department of Chemistry, Faculty of Science, Ochanomizu University, 2-1-1 Otsuka, Bunkyo-ku, Tokyo 112-8610, Japan*
[c] *Molecular Structure Characterization Unit, RIKEN Center for Sustainable Resource Science, Wako, Saitama 351-0198, Japan*
[d] *South–Ukrainian National University, Staroportofrankovskaya str. 26, 65020, Odessa, Ukraine*
[e]*University of Helsinki, Faculty of Pharmacy, Viikinkaari 5E, 00014 Helsinki, Finland*

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A unique set of positional isomers of non-aggregating phthalocyanines has been isolated and described, and their complexes with Co(II), Pd(II) and other metals were prepared. [1] The positional isomers (C_{4h} denoted "windmill", C_{2v} "frog" and C_S "dragon") differ substantially in their NMR, optical, and electrochemical properties, which makes them an excellent testbed for probing the computational chemistry tools and optimization of the computational modelling. Due to their non-aggregating nature even as Co(II) complexes, the synthesized molecules also make an excellent system for paramagnetic NMR studies, allowing for precise mapping of the proton relaxation times and H/C chemical shifts depending on the proximity to the paramagnetic Co(II). We achieved a nearly complete description of chemical shifts and longitudinal relaxations at distances 4 to 12 Å from the paramagnetic cobalt atom in the centre of the macrocore.

We managed to enhance the yield of sterically constrained frog and dragon isomers by a metal-templated tetramerization of phthalonitrile with further demetallation into phthalocyanine freebases. This allowed for a selective optimized synthesis of Pd derivatives of all three isomers and their comparative studies for a photodynamic action. Even though all three molecules demonstrated a high yield of the singlet oxygen, their ability for a light-triggered drug release from the liposomal carriers was significantly different. The frog and dragon isomers were most efficient for in the photodynamic cargo release, because of their enhanced ability to incorporate into the lipid bilayers.

The non-aggregating nature of α-(di*tert*butylphenyl)-substituted phthalocyanines also allows them to preserve their spectral properties in a solid state, even in smeared unordered films. When crystallised, especially the windmill isomer forms MOF-like molecular crystals with nanocavities within, which might be useful for various catalytic reactions.

REFERENCES

1. Efimov *et al.*, *Phys. Chem. Chem. Phys.* **2024**, 26, 18113

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Design and Application of Aerogel-based Catalysts for the Oxygen Reduction Reaction in Fuel Cells

Lior Elbaz

Bar-Ilan University, Ramat Gan 5290002, Israel

Among the key physical and chemical properties required from catalysts and catalysts' supports for fuel cell and water electrolyzers are high surface area and electronic conductivity. These have been limiting factors in the design of advanced materials for energy production and storage. In the past decade we have been focusing my research on designing advanced 3D materials' frameworks based on aerogels.

During these years, we developed three main categories of aerogel-based materials for fuel cells and water electrolyzers: inorganic covalent frameworks, metal oxides, and ceramics. These have been used for catalyzing the oxygen reduction reaction in fuel cells, the oxygen evolution and hydrogen evolution reactions in water electrolyzers and hydrogen pumps, and as corrosion-resistant catalysts' supports in fuel cells. In this talk I will share our journey in the development of inorganic covalent aerogels, based on porphyrins, phthalocyanines and corroles, from the design criteria, synthesis and application of some of the state of the art catalysts for oxygen reduction in fuel cells.

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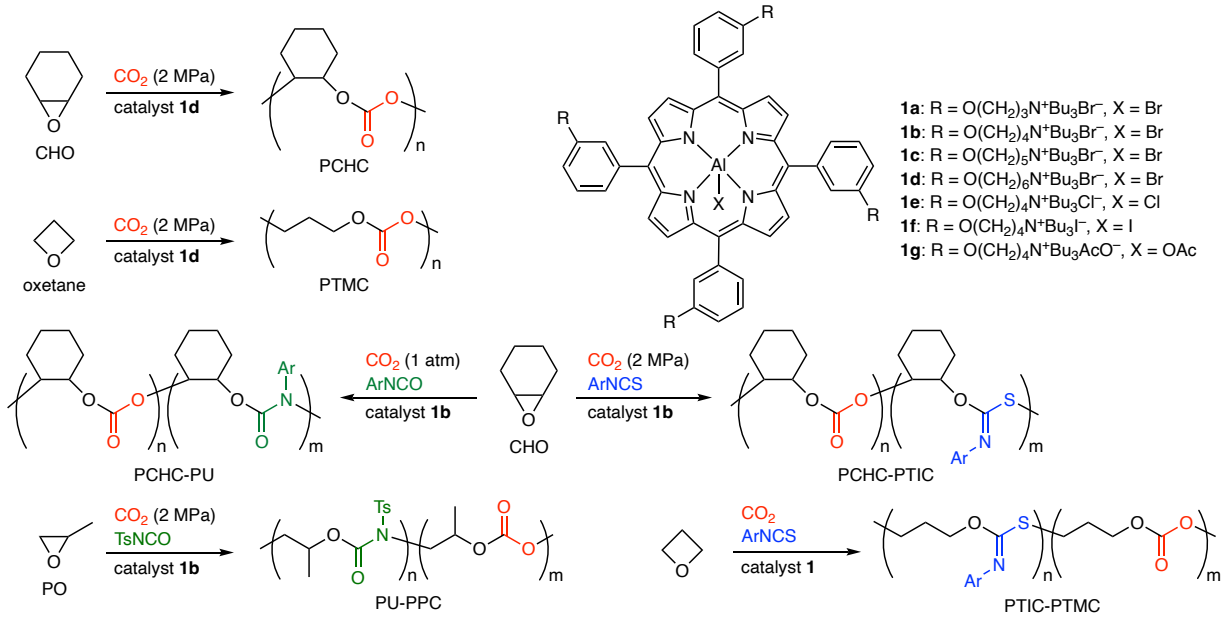
Synthesis of CO_2-Based Polymers Using Bifunctional Porphyrin Catalysts

Tadashi Ema

Okayama University

ORALS

Synthesis of cyclic carbonates or polycarbonates from epoxides or oxetanes and CO_2 is important from the viewpoint of green chemistry. The catalysts play a key role in the promotion of these reactions, and we have developed bifunctional metalloporphyrin catalysts capable of catalyzing these reactions efficiently.[1] In this presentation, we will focus on the copolymerization of epoxides or oxetanes and CO_2 for the synthesis of polycarbonates [2,3] and the terpolymerization of epoxides, CO_2, and the third monomers (Scheme 1).[4,5] The latter is useful for not only the creation of new CO_2-based polymers but also the tuning of the physical and chemical properties of the resulting polymers.[6]



Scheme 1. Synthesis of various CO_2-based polymers using bifunctional porphyrin catalysts.

REFERENCES

1. Ema, T. *Bull. Chem. Soc. Jpn.* **2023**, *96*, 693–701.
2. Deng, J.; Ratanasak, M.; Sako, Y.; Tokuda, H.; Maeda, C.; Hasegawa, J.; Nozaki, K.; Ema, T. *Chem. Sci.* **2020**, *11*, 5669–5675.
3. Maeda, C.; Inoue, H.; Ichiki, A.; Okihara, T.; Ema, T. *ACS Catal.* **2022**, *12*, 13042–13049.
4. Maeda, C.; Kawabata, K.; Niki, K.; Sako, Y.; Okihara, T.; Ema, T. *Polym. Chem.* **2023**, *14*, 4338–4343.
5. Nakaoka, K.; Muranaka, S.; Yamamoto, I.; Ema, T. *Polym. Chem.* **2024**, *15*, 707–713.
6. Nakaoka, K.; Ema, T. *Chem. Commun.* **2025**, *61*, 46–60.

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Designing Porphyrin Derivatives for Antimicrobial PDT

Ana S.M. Joaquinito[a], Cátia Vieira[b], Cristina J. Dias[a], Carlos J.P. Monteiro[a], Maria Bartolomeu[b,c], Nuno M.M. Moura[a], M. Amparo F. Faustino[a]

[a] *LAQV-REQUIMTE & Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal*
[b] *CESAM & Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal*
[c] *Centre for Interdisciplinary Research in Health (CIIS), Universidade Católica Portuguesa, Faculty of Dental Medicine, 3504-505, Viseu, Portugal*

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Porphyrins are tunable tetrapyrrolic compounds whose photophysical and biological properties can be controlled through molecular design. Peripheral functionalisation, charge distribution, and π-system extension strongly influence light absorption, singlet oxygen generation, and interactions with biological systems.
This presentation will focus on porphyrins developed for health-related applications, specifically antimicrobial PDT, linking structural modifications to photophysical characterisation and antimicrobial performance to identify the features governing light-induced microbial inactivation. [1-4]

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REFERENCES

1. Mendes A.C., Moura N.M.M., Faustino M.A.F., Neves M.G.P.M.S., Chronakis I.S., "Porphyrin-based electrospun nanomaterials for life science applications" *BBA Advances*, **2025**, 7, 100160, https://doi.org/10.1016/j.bbadva.2025.100160
2. Chaves I., Morais F., Vieira C., Bartolomeu M., Faustino M. A. F, Neves M. G. P. M. S., Almeida A, Moura N. M. M.,Can porphyrin-triphenylphosphonium conjugates enhance the photosensitizer performance towards bacterial strains? *ACS Applied Bio Materials*, **2024**, 7(8): 5541–5552 https://doi.org/10.1016/j.inoche.2025.114426
3. Bartolomeu M., Monteiro C.J.P., Fontes M., Neves M.G.P.M.S., Faustino M.A.F., Almeida A. Photodynamic inactivation of microorganisms in different water matrices: The effect of physicochemical parameters on the treatment outcome, *Science of the Total Environment*, **2023**, 860, 160427. http://dx.doi.org/10.1016/j.scitotenv.2022.160427
4. Lopes P., Joaquinito A.S.M., Ribeiro A., Moura N.M.M., Gomes A.T.P., Guerreiro S.G., Faustino M.A.F., Almeida A., Ferreira P., Coimbra M.A., Neves M.G.P.M.S., Gonçalves I., Starch-based films doped with porphyrinoidphotosensitizers for active skin wound healing, *Carbohydrate Polymers*, **2023**, 313, 120894. https://doi.org/10.1016/j.carbpol.2023.120894

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Stereoselective carbene transfer reactions with pyridotriazoles catalyzed by engineered hemoproteins

Rudi Fasan,[a] Satyajit Roy,[a] Yining Wang,[a] Mary Siriboe,[a] Alistair Sterling,[a] Yong Zhang,[b]

[a] *Department of Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, TX 75080, United States.*
[b] *Department of Chemistry and Chemical Biology, Stevens Institute of Technology, Hoboken, NJ 07030, United States*

Transition metal-catalyzed carbene transfer reactions are powerful strategies for the construction of new carbon-carbon and carbon-heteroatom bonds. Recent progress by our group and others have demonstrated that heme-containing proteins and enzymes, including (myo)globins, cytochromes P450, cytochrome *c*, and dehaloperoxidase, can be repurposed as versatile biological catalysts for mediating carbene transfer reactions that do not occur in nature.[1-4] Despite this progress, the scope of these transformations has been largely restricted to diazo compounds as carbene precursor reagents, limiting the range of compounds that can be synthesized through this strategy. Here, we report the development and investigation of engineered hemoprotein-based catalysts for stereoselective carbene transfer reactions with pyridotriazoles, an attractive yet underexplored class of carbene donor reagents. These methodologies provide access to new classes of enantioenriched pyridine-containing cyclopropanes and α-pyridyl sulfides of high value for medicinal chemistry and other applications. Mechanistic studies provide insights into the mechanism of these novel transformations, revealing an intriguing ability of these systems to exhibit multi-state reactivity in carbene transfer chemistry.

REFERENCES

1. O. F. Brandenberg, R. Fasan, F. H. Arnold. *Curr. Opin. Biotechnol.* **2017**, *47*, 102-111.
2. M. G. Siriboe, R. Fasan, *Bull. Jpn. Soc. Coord. Chem.* **2022**, *80*, 4-13.
3. X. Ren, R. Fasan, *Curr. Opin. Green Sustain. Chem.* **2021**, *31*, 100494.
4. Z. Liu, F. H. Arnold, *Curr. Opin. Biotechnol.* **2021**, *69*, 43-51.

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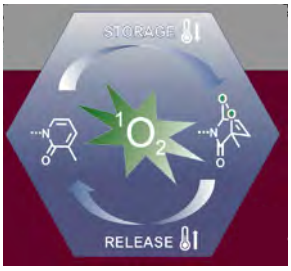
Remote Photosensitzation with SubPc/BOIMPY-Pyridone Dyads

Rüdiger Faust, Anika Petersen and Lorena Vogt

University of Kassel, Institute for Chemistry and CINSaT – Center for Interdisciplinary Nanostructure Science and Technology, Heinrich-Plett-Str. 40, 34132 Kassel, Germany, r.faust@uni-kassel.de

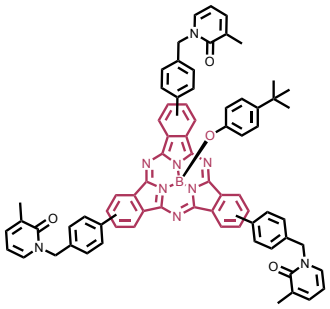
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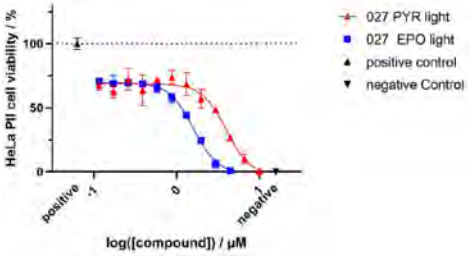
We are currently investigating photophysical dyads composed of a photosensitizer and covalently attached singlet-oxygen catch-and-release units. To this end we have synthesized pyridinone-modified SubPc and BOIMPYs derivatives, relying on the reversible endoperoxiode formation of pyridinone with singlet-oxygen. We have rigorously characterized their photophysical behaviour of the sensitizers' pyridinone forms and the thermochemistry of the corresponding endo forms. Furthermore, we have synthetically varied the number and position of the pyridinone units with respect to the photosensitizing cores.

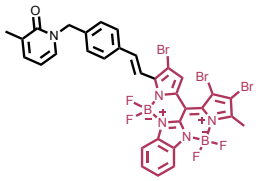


The biological activity of the SubPc-pyridinone dyad was explored in HeLa cell assays and significant phototoxicity was observed for both forms.

This research will be extended to supramolecular binding motives to provide for the dynamic and reversible attachment of the singlet-oxygen carrier unit. Progress of this ongoing research will be reported.







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Symmetry-Breaking Charge Separation Processes in Phthalocyanine-Based Systems

Fernando Fernández-Lázaro,[a] Jorge Follana-Berná,[a] Nathalie Zink-Lorre,[a] Ángela Sastre-Santos,[a] Andrew W. Dawson,[b] Francis D'Souza[b]

[a] *Área de Química Orgánica, Instituto de Bioingeniería, Universidad Miguel Hernández, Elche 03202 (Alicante), Spain. E-mail: fdofdez@umh.es*
[b] *Department of Chemistry, University of North Texas, Denton, Texas 76203-5017, USA.*

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Among all the possible structures that can be built by covalently linking simpler molecules, the specific pairing of identical chromophores is gaining attention due to the possibility to generate photoinduced symmetry-breaking charge separation (SB-CS) processes [1]. In such systems, the excited state of the dimer is effectively broken by molecular vibrations or fluctuations in the surrounding dielectric medium, thus generating a charge-separated state where the initially identical chromophores now posess opposite electrical charges.
One of the chromophores that have been commonly used in the symmetry-breaking processes are phthalocyanines (Pcs) due to their photostability and far-red light absorption [2].
In this communication, we will present the synthesis of novel systems for SB-CS, like the Pc-based one depicted in Figure 1, where the azo moiety allows to control the distance between the Pc subunits. The effect of the *inter*-Pc distance in the SB-CS process will be disclosed

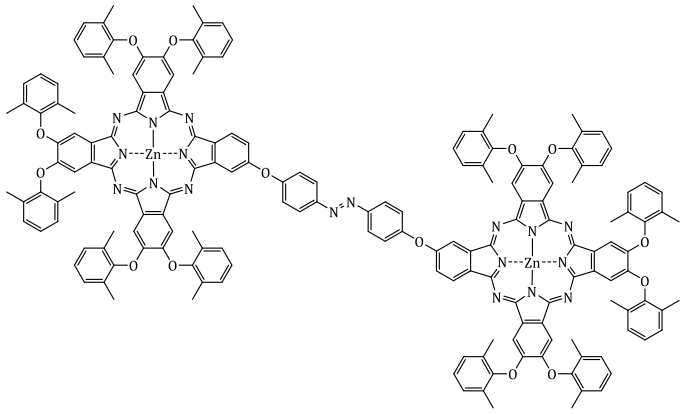


Figure 1. ZnPc-azo-ZnPc triad for symmetry-breaking charge transfer studies.

REFERENCES

1. V. Markovic, D. Villamaina, I. Barabanov, L. M. Lawson Daku, E. Vauthey, *Angew. Chem. Int. Ed.* **2011**, *50*, 7596–7598.
2. G. Bottari, G. de la Torre, D. M. Guldi, T. Torres, *Chem. Rev.* **2010**, *110*, 6768–6816.

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Switchable Formation of Triplet States in BODIPY via Charge Transfer: Toward Next-Generation Photosensitizers

Mikhail A. Filatov[a]

[a]*Technological University Dublin, City Campus, Grangegorman, Dublin, D07ADY7, Ireland*

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Triplet photosensitizers are indispensable for diverse photochemical applications. Traditionally, their design has relied on the introduction of heavy atoms, such as transition metals or halogens, into organic dyes to enhance spin–orbit coupling and facilitate intersystem crossing (ISC). While effective, this approach introduces several drawbacks, including high cost, toxicity, and reduced triplet excited-state lifetimes. An alternative mechanism that avoids the need for heavy-atom insertion is spin–orbit charge transfer intersystem crossing (SOCT-ISC), where photoinduced electron transfer within a donor–acceptor system generates a charge-transfer (CT) state that can recombine into the triplet manifold. Because the energy and lifetime of the CT state are highly sensitive to environmental parameters such as solvent polarity and viscosity, the balance between fluorescence and ISC can be modulated by the surrounding medium, enabling external control over excited-state dynamics.

BODIPY donor–acceptor dyads provide a highly adaptable platform for SOCT-ISC due to their tunable redox potentials and excited-state energies, which can be precisely adjusted through substitution of the pyrrolic core. Heavy-atom-free BODIPY sensitizers combine low toxicity, long triplet lifetimes, and structural modularity.[1] In these systems, the excited-state behaviour can be switched reversibly between fluorescence emission and triplet-state generation. We define this behaviour as switchable ISC (sISC), where the competition between radiative and non-radiative decay pathways is governed by local environmental factors. This feature enables the rational design of sensitizers with a desired ratio between fluorescence and singlet oxygen generation, useful for bioimaging, sensing, and photodynamic therapy applications.[2]

New BODIPY sensitizers have also been shown to enhance triplet–triplet annihilation upconversion (TTA-UC) efficiency due to their long triplet lifetimes (up to several hundred microseconds). Moreover, the switchability of ISC in these dyes allows them to function both as sensitizers and emitters, expanding the scope of upconversion systems.[3] Most recently, we optimized their performance in the photopolymerization of acrylate monomers, developing new BODIPY donor–acceptor sensitizers that outperformed conventional heavy-atom-containing sensitizers in photopolymerizable materials. These systems enabled holographic recording of diffractive structures and fabrication of optical devices for light management.[5] This presentation will highlight recent advances in the design and application of BODIPY dyes exhibiting SOCT-ISC, emphasizing their switchable photophysical properties and multifunctionality across biomedical and optical material fields.

REFERENCES

1. M. A. Filatov, *Org. Biomol. Chem.* **2020**, *18*, 10.
2. A. Sheehan, I. A. Okkelman, G. Groslambert, C. Bucher, R. I. Dmitriev, M. A. Filatov, *Chem. Eur. J.* **2025**, 31, e202404188.
3. N. Kiseleva, M. A. Filatov, J. C. Fischer, M. Kaiser, M. Jakoby, D. Busko, I. A. Howard, B. S. Richards, A. Turshatov, *Phys. Chem. Chem. Phys.* **2022**, *24*, 3568.
4. A. Sheehan, T. Mikulchyk, C. S. P. De Castro, S. Karuthedath, W. Althobaiti, M. Dvoracek, Sabad-e-Gul, H. J. Byrne, F. Laquai, I. Naydenova, M. A. Filatov, *J. Mater. Chem. C* **2023**, *11*, 15084.
5. M. A. Filatov, T. Mikulchyk, M. Hodée, M. Dvoracek, V. N. K. Mamillapalli, A. Sheehan, C. Newman, S. M. Borisov, D. Escudero, I. Naydenova, *J. Mater. Chem. C* **2025**, *13*, 6993.

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Anchor-Driven Assembly

Amar H. Flood

Indiana University

Molecular recognition provides an essential understanding of non-covalent interactions between molecules and provides a basis for self-assembly. They can be used in the stabilization of reactive species, particularly when the key recognition involves guests of high value. Porphyrins are exemplary of these recognition targets as they serve important roles across chemistry, biology, and material science. For instance, proteins are the hosts that co-assemble with porphyrins to enable the transport of oxygen. The recognition of porphyrins in synthetic systems has historically relied on ligands that coordinate to the metal center with more recent encapsulation inside molecular cages. Here, we describe the discovery of a new mode of porphyrin binding in which the axial ligand serves as a recognition anchor. The anchor was found to be complementary to the anion-binding cavity of using cyanostar macrocycles despite the overall net charge being neutral. This synthetic host bears 10 CH hydrogen bond donors focused into the cavity to bind the anchor (A) group on the porphyrin. Recognition is mediated by the steric and electronic availability of the lone pairs on the axial ligand, and benefits from pi stacking between macrocycles. This new mode of assembly with porphyrins, its functions, and its extensions will be described.

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Computationally Assisted Design of Heme Binding Self-Assembled Peptide Materials

H. Christopher Fry, Jesse Prelesnik, Henry Chan

Center for Nanoscale Material, Argonne National Laboratory

Anaerobic bacteria like Geobacter sulfurreducens utilize long aspect ratio heme binding protein fibers to carry out long range electron transfer as part of their respiratory process. These fibers can be harvested and utilized as biomolecular electronic materials because they were discovered to be electronically conductive. Inspired by this phenomenon and material application, we aim to develop a library of heme binding self-assembled peptide materials to establish design criteria. Through empirical design of amphiphilic peptides, success has been found. Examples of these achievements like long aspect ratio nanofibers and bilayer assemblies that contain heme will be shared in detail. It is of great note, however, that the design strategies are heavily biased towards researcher intuition. To expand the understanding of heme binding self-assembled peptides, the combination of experimentation, molecular dynamic simulation, and machine learning strategies offers a unique opportunity to explore the vast sequence space of peptide design (often referred to as the 20^n problem where 20 represents the canonical amino acids and n represents the number of amino acids in the peptide sequence). In this presentation, successes and limitations and future directions of the computation/experimentation collaboration will be discussed.

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From porphyrin to functional imide π-systems for organic electronics

Norihito Fukui[a]

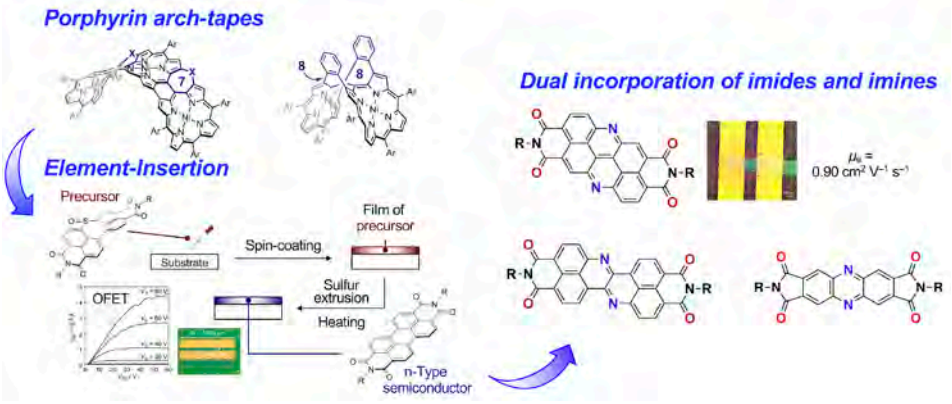
[a] *Department of Molecular and Macromolecular Chemistry, Graduate School of Engineering, Nagoya University, Aichi, Japan*

ORALS

During my Ph.D. studies at Kyoto University under the supervision of Prof. Osuka, I synthesized non-planar fused porphyrin oligomers, named as porphyrin arch-tapes.[1] The key to achieving curvature in these structures was the conceptual insertion of atoms between porphyrin units, which induced structural distortion.

I began my academic career in 2018 and subsequently launched a new project applying this element-insertion strategy to perylene bisimide (PBI), a versatile component in materials science. PBI is particularly promising as an n-type semiconductor. However, its low solubility in common organic solvents necessitates vacuum deposition for film fabrication, despite the growing demand for printable electronics. To address this challenge, I developed a sulfur-insertion strategy to design soluble PBI precursors.[2] The resulting sulfur-inserted PBIs exhibited high solubility due to their non-planar structures. Upon heating, these molecules underwent sulfur-extrusion reactions, quantitatively yielding PBI. This enabled the fabrication of n-type semiconductor films via solution processing, using spin-coating followed by thermal treatment.

In the course of this research, I also synthesized several imide-substituted nitrogen-containing π-systems.[3] These molecules demonstrated exceptionally high electron affinity, attributed to the dual incorporation of imide groups and imine-type nitrogen atoms, making them effective n-type semiconductors. Notably, acridino[2,1,9,8-*klmna*]acridine bisimide exhibited a brickwork-type packing alignment in its crystal structure. Photoconductivity measurements suggested that its intrinsic electron mobility follows a band-transport model. Accordingly, a single-crystal organic field-effect transistor (OFET) device based on this compound achieved an electron mobility of 0.90 $cm^2 V^{-1} s^{-1}$.



REFERENCES

1. (a) *J. Am. Chem. Soc.* **2017**, *139*, 9075; (b) *Angew. Chem. Int. Ed.* **2018**, *57*, 6304; (c) *Bull. Chem. Soc. Jpn.* **2018**, *91*, 1131.
2. (a) *J. Am. Chem. Soc.* **2020**, *142*, 11663; (b) *J. Am. Chem. Soc.* **2024**, *146*, 29383.
3. (a) *Angew. Chem. Int. Ed.* **2021**, *60*, 14060; (b) *Chem. Sci.* **2023**, *14*, 635; (c) *J. Mater. Chem. C* **2025**, *13*, 655; (d) *JACS Au* **2025**, *5*, 1421.

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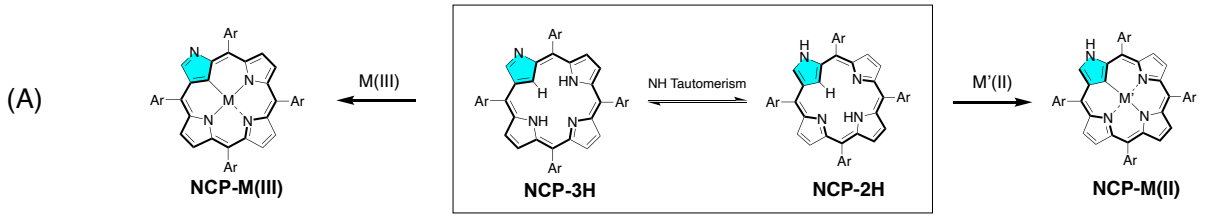


Electronic and magnetic interactions between N-confused porphyrin dimers

Hiroyuki Furuta[a,b]

[a]*Center for Supramolecular Chemistry and Catalysis, Department of Chemistry, College of Sciences, Shanghai University, Shanghai 200444, P. R. China*
[b]*Department of Applied Chemistry, Graduate School of Engineering, Kyushu University, Fukuoka 819-0395, Japan. (E-mail: furuta.hiroyuki.165@m.kyushu-u.ac.jp)*

The aromaticity of the planar porphyrinoids is usually controlled by the number of electrons in the π-conjugated circuits and is readily altered by modulating the π-circuits upon oxidation, reduction, ring-fusion, ring expansion, core-modification, etc. In the N-confused porphyrin case, the π-conjugation pathways can be modulated by NH tautomerism (**NCP-3H** and **NCP-2H**).[1] The circuits can be controlled by metalation (e.g., **NCP-M(III)** and **NCP-M(II)**). The α-position of the confused pyrrole ring could serve as a turnout point of the π-conjugation pathways, and the outward-pointing N atom serves as the hydrogen bonding and metal coordination site.[2] In this presentation, the peculiar role of the N-confused pyrrole ring for electron and magnetic interactions between two porphyrin rings will be discussed using several dimeric N-confused porphyrin systems.[3]



REFERENCES

1. a) H. Furuta, T. Ishizuka, A. Osuka, A. Dejima, H. Nakagawa, Y. Ishikawa, *J. Am. Chem. Soc.* **2001**, *123*, 6207. b) T. Ishizuka, R. Sakashita, O. Iwanaga, T. Morimoto, S. Mori, M. Ishida, M. Toganoh, K. Takegoshi, A. Osuka, H. Furuta, *J. Phys. Chem*. **2020**, *124*, 5756.
2. M. Toganoh, H. Furuta, *Chem. Rev.* **2022**, *122*, 8313.
3. a) M. Toganoh *et al*. *Chem. Lett.* **2011**, *40*, 1021. b) K. Yamasumi *et al.*, *Chem. Eur. J*. **2020**, *26*, 13590. c) K. Yamasumi *et al.*, *J. Porphyrins Phthalocyanines* **2021**, *25*, 447. d) O. Iwanaga *et al.*, *RSC Adv.* **2021**, *11*, 24575; e) O. Iwanaga *et al.*, *J. Porphyrins Phthalocyanines* **2023**, *27*, 1074.

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Development of Near-Infrared Light-Responsive Phthalocyanine-Based Photocatalysts

Taniyuki Furuyama[a]

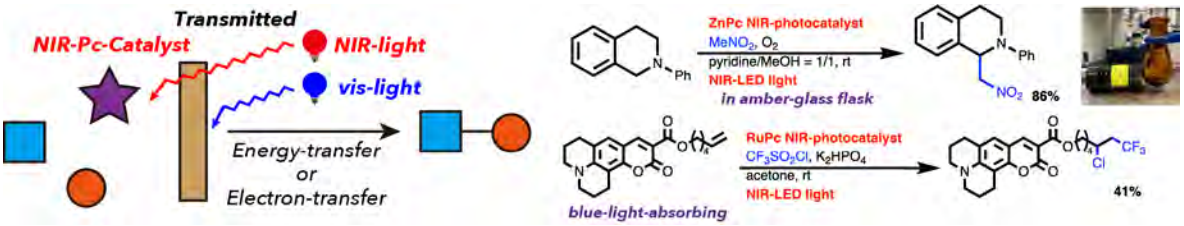
[a]*Graduate School of Engineering, University of Hyogo, 2167 Shosha, Himeji, 671-2280, Japan (furuyama@eng.u-hyogo.ac.jp)*

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Light energy is an attractive alternative to conventional thermal energy for driving molecular transformations. Although visible-light-mediated reactions have been widely investigated, they often face challenges such as limited penetration depth and uncontrolled activation when using visible-light-absorbing substrates. By contrast, the use of red-to-near-infrared (NIR) light offers high transparency and enables selective reactions under shielded conditions. Phthalocyanine (Pc) derivatives are ideal platforms for these applications because their optical and redox properties can be precisely tuned by modifying the central element and peripheral substituents.[1]

In this presentation, we describe our recent progress in the development of Pc-based photocatalysts for low-energy light utilization. By introducing a metal into the central core of Pc, an excited triplet state is efficiently generated via the heavy-atom effect. We developed a Pc ruthenium complex-catalyzed trifluoromethylation reaction using 634 nm-red light. Although the chlorotrifluoromethylation of simple alkenes with CF_3SO_2Cl proceeded in high yields,[2] styrene derivatives initially produced complex mixtures. After optimizing the reaction conditions, successful bifunctionalization of styrene derivatives was achieved using the Umemoto reagent as the CF_3 source in the presence of various nucleophiles.[3] Mechanistic studies confirmed that these reactions proceed via an electron-transfer pathway. Furthermore, we focused on the energy-transfer reaction with oxygen to enable the use of longer wavelengths. Using a Pc zinc complex catalyst, an 810 nm-NIR light-driven cross-dehydrogenative coupling reaction of tetrahydroisoquinolines with nucleophiles was realized.[4] Furthermore, we expanded this system to the direct modification of π-skeletons by generating aryl radicals from arylhydrazine derivatives, enabling the introduction of phosphorus, sulfur, and boron functional groups into aromatic rings under NIR-light irradiation.[5]

These results demonstrate the significant utility of NIR light, allowing for transformations in shielded environments or on substrates that absorb visible light. Our findings indicate that Pc derivatives are effective for the design of catalysts for wavelength-selective molecular transformations using low-energy light.



REFERENCES

1. *J. Porphyrins Phthalocyanines* **2022**, *26*, 790–806.
2. *Chem. Commun.* **2021**, *57*, 13594–13597.
3. *J. Org. Chem.* **2024**, *89*, 8178–8184.
4. *Chem. Eur. J.* **2022**, *28*, e202103223.
5. *J. Org. Chem. in press.*

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Porphyrin-based Nanostructures characterized by means of computational simulations

Aurelio Gallardo[a]

[a]*IMDEA Nanociencia, C/ Faraday 9, Campus de Cantoblanco, Madrid, 28049*

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On-surface chemistry is a rapidly growing field that enables the synthesis of molecular structures that are not accessible via traditional wet chemistry. In this context, high-resolution scanning probe microscopy techniques can provide unprecedented spatial resolution, enabling precise identification of individual reaction products. Nevertheless, a deep understanding of the reaction mechanism under the substrate-imposed conditions remains unknown.

In this context, various computational strategies are available to characterize the optimal reaction pathways of chemical processes occurring on the surfaces of solids. For example, the nudged elastic band (NEB) is one of the most popular approaches, as are various transition state theory methods beyond it. These approaches have demonstrated their capability to characterize the potential energy landscape of the reaction pathways [1-2]. Another approach that attracts the interest of the on-surface synthesis community is the application of molecular dynamics (MD) methods in the canonical ensemble, using QM/MM (quantum mechanics/molecular mechanics) for interatomic forces [3-5]. This approach, which combines Density functional theory (DFT) and empirical force fields to describe interaction forces, enables the simulation of very large systems at very low computational cost while still accounting for the crucial quantum-mechanical interactions. Also, such temperature-dependent simulations include the effect of entropy, vibrational modes, concerted motion, etc.

I will present experimental and computational results from different projects in which we use these computational approaches to better understand the group's experiments on the on-surface synthesis of porphyrinoid-based one- and two-dimensional nanostructures. For example, the synthesis of hemiporphyrinoid-based nanostructures via [3+3] cycloatomatization and the Co-metalation of their chemical pocket, showing a low coordination with the captured ion. [1] Another example is our recently submitted study on the expansion of the chemical pocket of porphyrin macrocycles into 20-π free-based, highly antiaromatic expanded porphyrinoids, opening new possibilities for tuning their electronic properties. We characterized these systems using a combination of computational and experimental SPM (Scanning Probe Microscopy) techniques, DFT simulations of their electronic structure, and DFT-based characterization of the expansion reaction mechanism.

These examples, together with our most recent results in the tailoring of molecular nanostructures, will illustrate the power of our computational approaches to help us understand the chemistry and physics behind the On-surface reaction mechanism.

REFERENCES

1. The Role of Metal Adatoms in a Surface-Assisted Cyclodehydrogenation Reaction on a Gold Surface. J. Björk, et al. *Angew. Chem*., 61, e2022123.1-7 (2022).
2. Mechanisms of Halogen-Based Covalent Self-Assembly on Metal Surfaces. J. Björk, et al. *J. Am. Chem. Soc.* 135 (15) 5768–5775 (2013).
3. Strain-induced isomerization in one-dimensional metal–organic chains. M. Telychko *Angewandte Chemie* 131 (51), 18764-18770 (2019).
4. Designing highly delocalized solitons by harnessing the structural parity of π-conjugated polymers. K. Biswas, et al. *Nat. Synth.,* (2024).
5. On-Surface Synthesis of Covalently-Linked Carbaporphyrinoid-Based Low-Dimensional Polymers. A. Barragán, et al. *Small* 21 (2) 2408085 (2025).

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Carbene Transfer Reactions in Aqueous Environment Promoted by Heterogenized Iron Porphyrins

Emma Gallo[a], Matteo Cavalleri[a], Lucia Invernizzi[a] and Caterina Damiano[a]

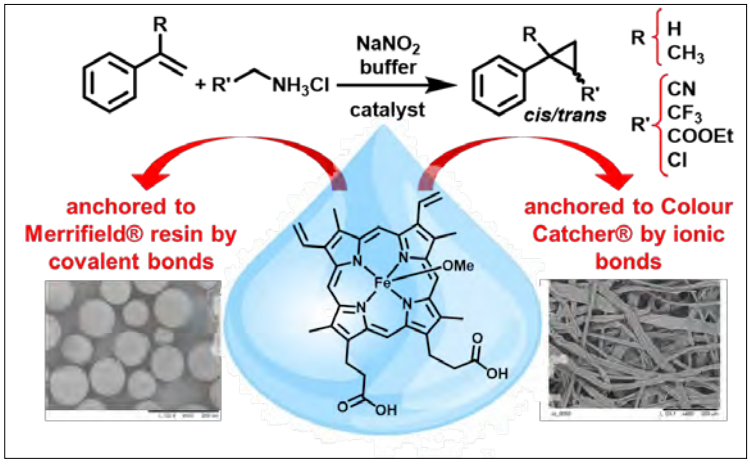
[a]*Department of Chemistry, Università degli Studi di Milano, Milan, Italy*

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Given the widespread use of metal porphyrin complexes in promoting carbene transfer reactions, [1] the development of heterogenized catalysts represents an important step toward greener and more environmentally friendly synthetic processes.

Herein, we present a methodology based on the use of heterogeneous catalysts that, when coupled with the generation of highly reactive carbene species in aqueous media, shows remarkable applicability to the synthesis of a wide class of substituted cyclopropanes.

The in-water diazotization/carbene generation/cyclopropanation protocol, previously reported by Morandi, Koenigs, and others, [2] was efficiently promoted by Fe(OMe)protoporphyrin IX catalyst supported either by covalent linkages onto Merrifield® Resin, or by ionic bonds onto Colour Catcher® material. The latter is a cellulose-based material commonly used in everyday life to capture dyes in laundry water and exhibits an excellent ability to strongly bind both free and metal porphyrins. The resulting material is fully biodegradable, exhibits strong performance in sensing and catalysis [3] and displays high thermal and chemical stability. Both heterogenized catalysts exhibited good activity in promoting the cyclopropanation of substituted alkenes, and their robustness allowed them to be recycled several times without significant loss of efficiency.



While the highest yields were obtained by using aminoacetonitrile hydrochloride as the carbene precursor, trifluoroethylamine hydrochloride led to the formation of the corresponding cyclopropanes with superior diastereoselectivities.

Optimization of the reaction conditions run in the presence of both Merrifield® Resin and Colour Catcher®-based catalytic materials revealed that catalytic performance was maximized in acetate buffer at pH 4.75.

REFERENCES

1. C. Damiano, L. Invernizzi, E. Gallo *Adv. Catal.* **2024**, *74*, 101; b) C. Damiano, P. Sonzini, A. Caselli, E. Gallo *Adv. Organomet. Chem*. **2021**, *76*, 145.
2. a) B. Morandi, J. Cheang, E. M. Carreira *Org. Lett.* **2011**, *13*, 3080; b) P. K. Mykhailiuk, R. M. Koenigs *Chem. Eur. J.* **2020**, *26*, 89; c) P. K. Mykhailiuk *Chem. Rev.* **2020**, *120*, 12718.
3. a) C. Damiano, A. Fata, M. Cavalleri, G. Manca, E. Gallo *Catal. Sci. Technol*., **2024**, *14*, 3996; b) C. Damiano, M. Cavalleri, C. di Natale, R. Paolesse, E. Gallo, *ChemistryEurope* **2023**, e202300020; c) F. Caroleo, G. Magna, C. Damiano, M. Cavalleri, E. Gallo, C. Di Natale, R. Paolesse, *Sens Actuators B Chem*. **2022**, 364, 131900.

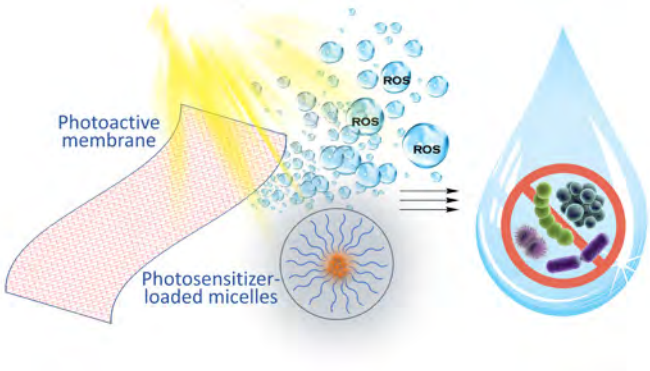
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Designing Photoactivity: Modulating Antimicrobial Photodynamic Effects through Polymer–Photosensitizer Interactions

Anzhela Galstyan,

[a]*University AffiliatioFaculty of Chemistry, Center for Nanointegration Duisburg-Essen (CENIDE), Center for Water and Environmental Research (ZWU) and Center of Medical Biotechnology (ZMB) University of Duisburg-Essen, Universitätsstr. 5, D-45141 Essen, Germany*

Photoactive polymer-based materials are emerging as versatile platforms for antimicrobial applications, offering light-controlled activity and tunable physicochemical properties. In this contribution, we present a comparative materials-chemistry perspective on polymer-supported photosensitizer systems, focusing on how polymer architecture and microenvironment govern photophysical behavior and functional performance. Using zinc phthalocyanines as model photosensitizers, we investigate both nanostructured polymer carriers and solid polymer matrices to elucidate general structure–function relationships relevant to photodynamic activity [1-3].



Schematic of a photosensitizer-loaded membrane and polymeric micelles generating reactive oxygen species under light to inactivate microorganisms.

Across different polymer platforms, the hydrophilic–hydrophobic balance, aggregation state of the photosensitizer, and local microenvironment are identified as key parameters controlling excited-state lifetimes and reactive oxygen species (ROS) generation under visible-light irradiation. Fluorescence lifetime measurements, including fluorescence lifetime imaging microscopy (FLIM), reveal pronounced spatial and temporal heterogeneities in excited-state dynamics, highlighting the presence of functionally distinct photoactive domains within heterogeneous polymer systems.

REFERENCES

1. F. Terlau, H. M. Martin, A. Galstyan, *Angew. Chem. Int. Ed.,* **2024**, e202414412.
2. A. Galstyan, *Chem. Eur. J.* **2024**, 30 (62), e202401305.
3. A. Galstyan, H. Majiya, U. Dobrindt, *Nanoscale Adv.*, **2022**, 4, 200-210.

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Self-Assembled Polar Multifunctional Materials

Miguel Garcia-Iglesias,[a] Victor Rodríguez,[a,b] David González-Rodriguez,[b] M. Kemerink[c]

[a]*QuIPRe Department, Nanomedicine-IDIVAL, University of Cantabria,*
[b]*Department of Organic Chemistry, Universidad Autónoma de Madrid*
[c]*Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg.*

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Recent advances in self-assembly and supramolecular chemistry enable precise bottom-up control over the structure and function of organic and polymeric materials, leading to dynamic, highly ordered nanostructures with unconventional and technologically relevant properties.Within this framework, we have designed and synthesized a new class of disc-shaped organic semiconductors [1] featuring dipolar side groups and a strong propensity to self-organize into columnar mesophases. These architectures simultaneously support ferroelectric coupling and quasi-one-dimensional charge transport As a result, ferroelectric polarization becomes strongly coupled to bulk electrical conductivity, leading to switchable and rectifying current–voltage characteristics. This behavior is particularly promising for the development of low-cost, non-volatile, rewritable memory devices (Figure 1). [2].

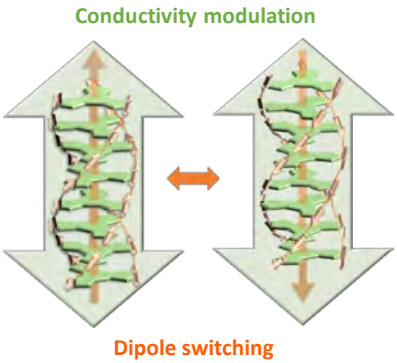


Figure 1. A cartoon of the coupling between ferroelectric polarization and conductivity

Building on this design strategy, we are currently exploring the fabrication of next-generation macro- and nanostructured organic photovoltaic devices (OPVs). These systems rely on self-assembled donor–acceptor conjugates that combine permanent dipole moments with efficient light-harvesting capabilities, opening new avenues for multifunctional organic optoelectronic materials [3].

REFERENCES

1. M. García-Iglesias, B. F. M. Waal, A. V. Gorbunov, M. Kemerink, E. W. Meijer, *J. Am. Chem. Soc.* **2016**, *138*, 6217-6223.
2. (a) A. V Gorbunov, M. García-Iglesias, J. Guilleme, T. D. Cornelissen, W. S. C. Roelofs, T. Torres, D. González-Rodríguez, E. W. Meijer, M. Kemerink, *Sci. Adv.* 2017, 3, e1701017. (b) N. M. Casellas, I. Urbanaviciute, T. D. Cornelissen, J. A. Berrocal, T. Torres, M. Kemerink, M. García-Iglesias, *Chem. Commun.* **2019**, *55*, 8828-8831.(c) L López-Gandul, A Fernández-Alarcón, N. M. Casellas, C. Naranjo, J Calbo, E. Ortí, M.García-Iglesias, L Sánchez. *Angew. Chem. Int. Ed.* **2025**,*64* e17603.
3. (a) J. Joseph, J. A. Berrocal, N. M. Casellas, D. M. Guldi, T. Torres, M. García-Iglesias, *J. Am. Chem. Soc.* **2024**, *146*, 30272−30280.

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Biological models for photoactivable nanoparticles and photosensitizers study

Magali Gary-Bobo[a]

[a] *IBMM, Univ Montpellier, CNRS, ENSCM, Montpellier, France*

Currently, the development of *in vitro* and *in vivo* models according to the 3Rs (reduction, replacement, refinement) is of great importance. Indeed, research activities need these robust and easy-to-use techniques to demonstrate the imaging and therapeutic potential of innovative nanoparticles and photosensitizers. Among several effective organic or inorganic nanoparticles, we are focusing on tunable nanoparticles offering several advantages in terms of drug or genetic material loading capabilities, photoactivatable properties for imaging or photodynamic therapy, and personalization for targeting. In our team, the biological effects of nanoparticles and photosensitizers are studied first on human cancer cell lines in culture and then on zebrafish embryos. The robustness of these models enables us to provide rapid and reliable proof-of-concept for biocompatible and therapeutic tools.

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Predicting NIR Phosphorescent Emission and Singlet Oxygen Sensitization by 5d Metalloporphyrins and Metallocorroles

Abhik Ghosh[a]

Department of Chemistry, UiT – The Arctic University of Norway, 9037 Tromsø, Norway

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Platinum porphyrins have long been known for their strong NIR phosphorescence, singlet oxygen sensitization, and photodynamic activity. In recent years, middle and late 5d transition metal corroles (involving Re, Os, Ir, Pt, and Au) have also been found to exhibit some or all of these attributes.[1] The phosphorescence quantum yields of 5d metallocorroles are generally lower, hovering around 1% and considerably lower for Ir corroles; several 5d metalloporphyrins also exhibit similarly low quantum yields or do not emit all. Similarly, while many 5d metallocorroles sensitize singlet oxygen formation, others do not.[2] Herein, we will present experimental measurements and DFT/TDDFT calculations on a wide range of 5d metalloporphyrins and metallocorroles in an effort to understand their divergent photophysical behavior.

REFERENCES

1. Alemayehu AB, Thomas KE, Einrem RF, Ghosh A. *Acc. Chem. Res*. 2021; **54**: 3095-3107.
2. Alemayehu AB, Conradie J, Larsen S, Pérez BCL, Settineri NS, Ghosh A.. Rhenium-Selenido Corroles: Reflections on 5d Metalloporphyrins and Metallocorroles as Triplet Emitters and Photosensitizers. *Inorg. Chem.* 2025; **64**: 12242-12253.

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Reactivity of High-Valent Iron Porphyrinoid Complexes

David P. Goldberg

Johns Hopkins University, Department of Chemistry, Baltimore, Maryland

High-valent iron porphyrinoid compounds are implicated in many synthetic catalytic and enzymatic reactions. Ring-contracted porphyrinoid complexes, such as iron corrolazines and corroles, offer valuable platforms for examining metal-ligand cooperativity and accessing unusual intermediates that are often challenging or impossible to characterize in a direct manner with conventional porphyrin scaffolds. This talk will focus on the synthesis and characterization of formally high-valent iron corrolazine and corrole complexes, either one or two electrons oxidized above the stable ferric oxidation state. Mössbauer, EPR, and UV-vis spectroscopic analyses are used to examine whether the oxidations are metal- or ligand-centered. The incorporation of oxo/hydroxo axial ligands will be described, and compared to non-oxo axial donors such as chloride. The reactivity of these species, such as in PCET reactions, will also be discussed.

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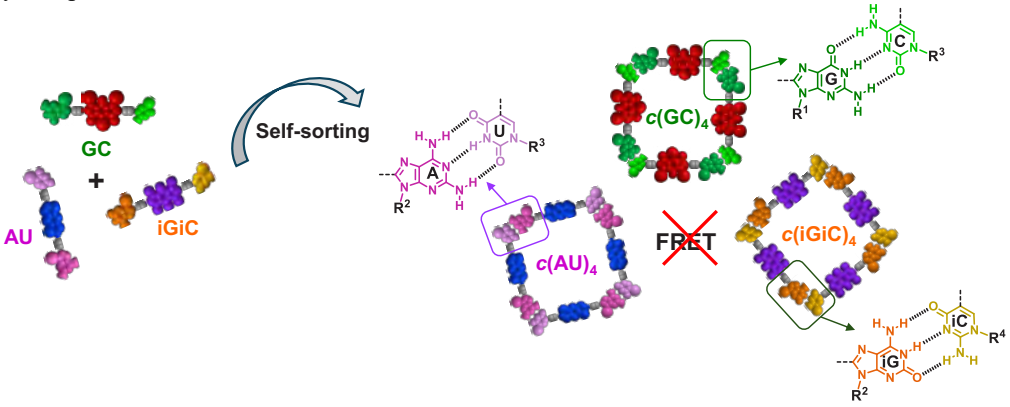
Investigating Watson-Crick Hydrogen-bonding using BODIPY Dye Probes

David González-Rodríguez,[a,b] **Marina González-Sánchez,**[a] **Jorge Rodrígez-Duran**[a]

[a] *Departamento de Química Orgánica, Facultad de Ciencias, Universidad Autónoma de Madrid, 28049 Madrid, Spain*
[b] *Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid Spain*

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A versatile strategy is described here to prepare cyclic systems whose size, shape, composition and function can be rationally predesigned and controlled at the nanoscale using concepts and tools of supramolecular chemistry. Cyclic tetramers[1] are formed from 4 monomeric π-conjugated subunits by Watson-Crick hydrogen-bonding interactions between nucleobase directors. A proper monomer preorganization affords high chelate cooperativities and thus high cyclization yields in solution[2,3] and onto surfaces.[4] Importantly, the use of BODIPY dys probes allowed us to demonstrate that only systems displaying sufficiently strong chelate cooperativity can achieve quantitative narcissistic self-sorting fidelities, either by dictating the distribution of cyclic species in complex mixtures or by ruling the competition between the intra- and intermolecular versions of a noncovalent interaction. A combination of 1D and 2D NMR, CD, and fluorescence spectroscopy with donor-acceptor FRET pairs, in diverse solvents and concentration ranges, clearly confirms the dominant role that chelate cooperativity can have in relatively complex mixtures.



REFERENCES

1. D. Serrano-Molina, A. de Juan, D. González-Rodríguez, *Chem. Rec.* **2021**, *21*, 480-497.
2. a) C. Montoro-García, J. Camacho-García, A. M. López-Pérez, M. J. Mayoral, N. Bilbao, D. González-Rodríguez, *Angew. Chem. Int. Ed.* **2016**, *55*, 223; b) C. Montoro-García, M. J. Mayoral, R. Chamorro, D. González-Rodríguez, *Angew. Chem. Int. Ed.* **2017**, *56*, 15649.
3. a) M. J. Mayoral, D. Serrano-Molina, J. Camacho-García, E. Magdalena-Estirado, M. Blanco-Lomas, E. Fadaei, D. González-Rodríguez, *Chem. Sci*. **2018**, *9*, 7809; b) D. Serrano-Molina, C. Montoro-García, M. J. Mayoral, A. de Juan, D. González-Rodríguez, *J. Am. Chem. Soc.* **2022**, *144*, 5450; c) M. González-Sánchez, D. Serrano-Molina,
4. N. Bilbao, I. Destoop, S. De Feyter, D. González-Rodríguez, *Angew. Chem. Int. Ed.* **2016**, *55*, 659.

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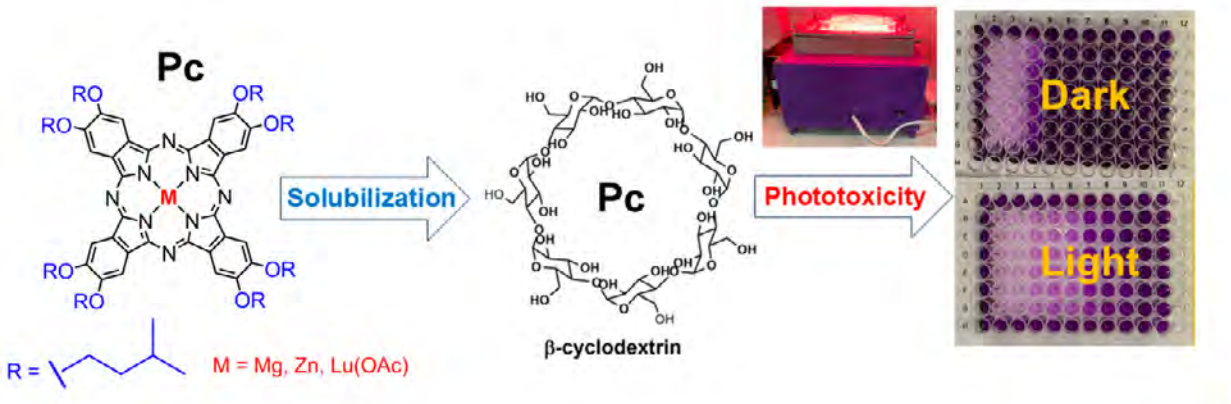
Isoamyloxy-substituted phthalocyanine complexes: synthesis, solubilization and photodynamic activity *in vitro*

Elena A. Gorbunova[a], Alina S. Agranat[a], Tatiana V. Dubinina[a]

[a] *Lomonosov Moscow State University, Department of Chemistry, 119991 Moscow, Russian Federation*

New photosensitizers based on isoamyloxy-substituted phthalocyanine complexes of Zn(II), Mg(II) and Lu(III) that exhibit photodynamic activity *in vitro* were described. Synthetic strategies were developed for commercially unavailable starting material 4,5-*bis*(isoamyloxy)phthalonitrile. A more efficient approach was found to involve alkylation of the OH groups of pyrocatechol with isoamyl bromide, electrophilic bromination and cyanation. Phthalocyanine zinc, magnesium and lutetium complexes were prepared by the metal template effect to facilitate the cyclization. Using the XANES method, coordination of the central ion by four nitrogen atoms was demonstrated for isoamyloxy-substituted zinc phthalocyanine.

The introduction of isoamyloxy groups leads to an increase in the fluorescence quantum yield of the corresponding magnesium complex compared to unsubstituted and aryloxy-substituted phthalocyanines described in the literature. Complexes of isoamyloxy-substituted phthalocyanines have demonstrated the ability to generate active oxygen metabolites: singlet oxygen and superoxide anion-radical. Successful encapsulation of hydrophobic phthalocyanines in β-cyclodextrin allowed obtaining water-soluble forms of the complex with a molar ratio of phthalocyanine to β-cyclodextrin of 1:1. The zinc complex showed the highest singlet oxygen quantum yield among the target complexes and, as a consequence, the best photodynamic effect *in vitro* (IC_{50} up to 2.16 μM), comparable to that of chlorin e6, an approved photodynamic therapy (PDT) photosensitizer.



We are grateful to the Russian Science Foundation No. 24-73-00062 for main support of this research.

REFERENCES

1. Gorbunova E.A. et al. // Inorganica Chimica Acta, 585 (2025) 122748.

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Self-Assembling of Cationic Phthalocyanines: from Type II to Type I Photodynamic Therapy

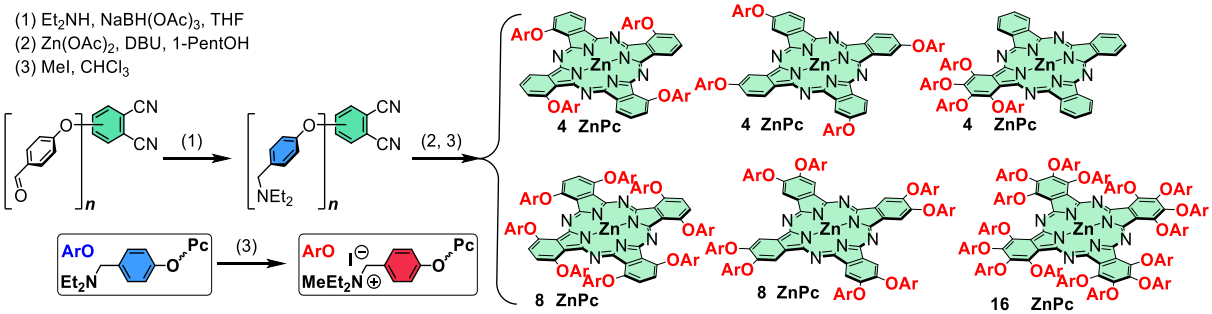
Yulia G. Gorbunova[a,b], Dmitry A. Bunin[a], Alexander G. Martynov[a], Aslan Yu. Tsivadze[a,b]

[a]*Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, Moscow, Russia*
[b]*Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, Moscow, Russia*

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Phthalocyanines are known to exhibit high photodynamic activity which strongly depends on their aggregation status in biological media [1]. In our work we study how self-assembling of cationic phthalocyanines affects their photobiological properties. With this aim, we elaborated novel and convenient approach for the synthesis of cationic phthalocyanines via reductive amination of 4-formylphenoxy-substituted phthalonitriles which afforded a library of water-soluble complexes with varying numbers and positions of cationic 4-(*N,N*-methyldiethylammoniummethyl)phenoxy substituents [2, 3]. We found that the substitution patterns allow to control the aggregation of complexes in aqueous media which allowed us to compare the photochemical and photobiological properties of purely monomeric and strongly aggregated photosensitizers.

Using a combination of chemical scavengers, we show that monomeric phthalocyanines predominantly generate singlet oxygen (Type II PDT), while their self-assembling switches their activity to Type I with generation of radical reactive oxygen species [4]. The Type I PDT is less dependent on oxygen concentration in the photosensitizer's microenvironment and proves to be more effective under conditions of tumor hypoxia, however disruption of Pc-based nanoparticles upon interaction with biomolecules [3] can reduce the therapeutic benefits of aggregation. We have shown that this limitation can be overcome by employing low-symmetry amphiphilic phthalocyanines as building blocks for nanoparticles, which show improved stability in physiological media and demonstrate Type I PDT pathway under simulated hypoxic conditions. Additionally, these nanoparticles acquire photothermal activity which broadens the scope of their therapeutic modalities.



Acknowledgement: this work was supported by Russian Science Foundation (grant № 24-13-00479).

REFERENCES

1. D. A. Bunin et al., *Biophys. Rev.*, **2023**, 15, 983–998.
2. D. A. Bunin et al., *Dyes Pigm.*, **2022**, 207, 110768.
3. D. A. Bunin et al., *J. Med. Chem.*, **2025**, 68, 658–673.
4. D. A. Bunin et al., *Opt. Mater.*, **2026**, 172, 117831.

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Functionalized and Non-functionalized Fluorophthalocyanines: Electronic and Symmetry Effects on Reactivity and Surface Anchoring

Marius Pelmuş, Alexander Y. Fadeev, and Sergiu M. Gorun

Department of Chemistry and Biochemistry, Seton Hall University, South Orange, NJ 07079, USA

Amino functionalization of electron-deficient phthalocyanines results in reduced reactivity, which is restored by blocking the N lone-pair exocyclic conjugation. While macrocycle functionalization may result in covalent anchoring on solid-state supports, the unfunctionalized perfluorinated materials can still be absorbed, a process favoured by intermolecular dipolar interactions that are a function of the phthalocyanine's symmetry and dictate their edge-on or face-on absorption configurations.

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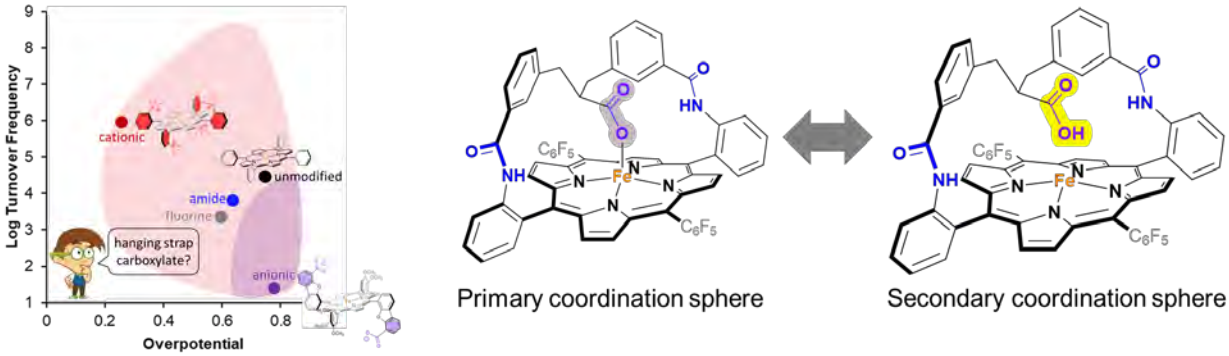
Turning Repulsion into Reactivity: A Dynamic Carboxylate Relay in Iron Porphyrin CO_2 Reduction

Philipp Gotico[a], Adrien Smith[b], Regis Guillot[b], Stéphane Le Gac, Winfried Leibl[a], Ally Aukauloo[b], Bernard Boitrel[c], Marie Sircoglou[b], Zakaria Halime[b]

[a]*Institut de Biologie Intégrative de la Cellule, CEA, 91191 Gif sur Yvette, France*
[b]*Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris Saclay, 91405 Orsay, France*
[c]*Institut des Sciences Chimiques de Rennes, Université Rennes 1, 35042 Rennes, France*

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Catalyst design increasingly draws inspiration from metalloenzymes, where precisely organized ligand environments around metal centers enable efficient capture and transformation of small molecules such as CO_2. While the primary coordination sphere governs redox properties, the secondary coordination sphere has emerged as a powerful lever for enhancing catalytic rates at low overpotentials through proton relays, hydrogen bonding, and electrostatic effects.[1] In CO_2 electroreduction, cationic secondary-sphere functionalities often promote reactivity, whereas anionic groups, such as sulfonates or carboxylates, are typically detrimental due to electrostatic repulsion of anionic metal–carboxylate intermediates.[2–4] Here, we report an exception: a precisely positioned "hanging" carboxylate embedded within an artificial distal pocket of an iron porphyrin catalyst using a rigid, preorganized strap.[5] Electrochemical, kinetic, and computational studies show that this carboxylate, in synergy with a trapped water molecule, enhances turnover frequencies by four orders of magnitude relative to a perfluorinated iron porphyrin at comparable low overpotential. This dramatic effect arises from proton-coupled electron transfer that induces transient protonation and dynamic repositioning of the carboxylate from the primary to the secondary coordination sphere, where it likely functions as a proton relay during CO_2 activation.



Scheme 1. Exploring unique reactivity of hanging carboxylates strapped in iron porphyrins.

REFERENCES

1. P. Gotico, W. Leibl, Z. Halime, A. Aukauloo, ChemElectroChem 2021, 8, 3472–3481.
2. I. Azcarate, C. Costentin, M. Robert, J.-M. Savéant, J. Am. Chem. Soc. 2016, 138, 16639–16644.
3. C. G. Margarit, C. Schnedermann, N. G. Asimow, D. G. Nocera, Organometallics 2019, 38, 1219–1223.
4. C. G. Margarit, N. G. Asimow, M. I. Gonzalez, D. G. Nocera, J. Phys. Chem. Lett. 2020, 11, 1890–1895.
5. A. Smith, P. Gotico, R. Guillot, S. Le Gac, W. Leibl, A. Aukauloo, B. Boitrel, M. Sircoglou, Z. Halime, Adv. Sci. 2025, 12, 2500482.

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On-Surface Chemistry of Porphyrins, Corroles, and Phthalocyanines

J. Michael Gottfried[a]

[a]*University of Marburg, Department of Chemistry, Hans-Meerwein-Strasse 4, 35043 Marburg, Germany*

Porphyrins, phthalocyanines, and corroles are versatile building blocks for surface functionalization due to their distinct (opto)electronic properties and reactivity. They readily form ordered monolayers that undergo metalation or transmetalation, ligand coordination, or intermolecular coupling. Here, the following aspects of the on-surface chemistry of porphyrins and related compounds will the presented: (1) Porphyrin monolayers and multilayers react with alkali metals, forming the corresponding dimetallic complexes with bipyramidal geometry. Formation of Li_2TPP proceeds via LiHTPP, which is stable can be isolated by sublimation [1]. Cs_2TPP is also thermally very stable and even desorbs intact from Ag(111) between 600 K and 750 K, allowing for its identification by mass spectrometry. Corroles form stable lithium complexes with up to four lithium atoms. In the open-shell Li_4 corrole complex, three lithium ions coordinate between neighboring nitrogens on one face of the macrocycle while the fourth lithium binds all four nitrogens on the opposite face. This geometry gives rise to a singly occupied molecular orbital formed by the overlapping 2s orbitals of the three cofacial lithium ions, collectively sharing one electron. (2) Transmetalation reactions of PbTPP on Cu(111) and Au(111) surfaces result in the formation of the corresponding Cu and Au complexes. The metal exchange is direct on the copper surface, while on the gold surface, the unmetalated 2HTPP occurs as an intermediate [2]. (3) Phthalocyanines, naphthalocyanines and their expanded homologs can be prepared by template-directed on-surface synthesis from suitable dinitrile-based precursors. These precursors also provide access to linear open-chain counterparts of phthalocyanines [3]. Structure, electronic properties and reactivities will be discussed based on extensive experimental and theoretical results. (4) Transition-metal porphyrin complexes on metallic substrates can form bivalent superstructures with quasi-periodic variation of the oxidation state of the metal center. This effect depends on the reactivity and structure of the substrate, as well as on coverage, and is related to adsorption sites. These studies showcase the rich on-surface chemistry of porphyrins and related macrocycles and highlight new opportunities for functional molecular architectures at interfaces.

REFERENCES

1. Maik Schöniger, Stefan R. Kachel, Jan Herritsch, J. Michael Gottfried, *A Monolithium Monohydrogen Porphyrin*, Angew. Chem. Int. Ed. 64, e202504928 (2025)
2. Jan Herritsch, Cong Guo, Lukas J. Heuplick, Mark Hutter, Qitang Fan, Florian Münster, Stefan R. Kachel, Malte Zugermeier and J. Michael Gottfried, *On-surface chemistry of Pb(II) tetraphenylporphyrin on Au(111): reversible metalation, thermal degradation, and formation of a covalent organic framework*, Phys. Chem. Chem. Phys. 27, 10875-10883 (2025)
3. Lukas J. Heuplick, Qitang Fan, Dmitriy A. Astvatsaturov, Tatiana V. Dubinina, J. Michael Gottfried, *On-surface synthesis of phthalocyanines with extended π-electron systems*, Comm. Chem. 7, 292 (2024).

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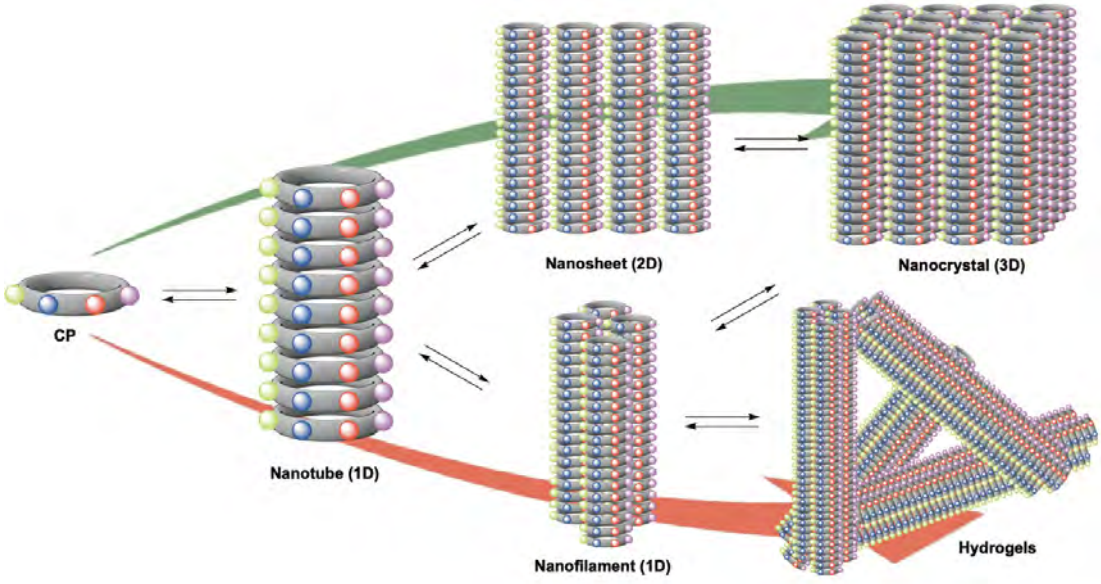
Self-Assembling Cyclic Peptides: Fibers and Nanosheets

Juan R. Granja, Alfonso Bayón-Fernández, Alba Torrón-Celada, Marcos Vilela-Picos, Martín Vázquez-Rodríguez

[a]*Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS) and Departamento de Química Orgánica. Universidade de Santiago de Compostela. Rúa de Jenaro de la Fuente, s/n, 15705, Santiago de Compostela, Spain.*

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Hierarchical self-assembly is a stepwise supramolecular process that forms complex structures from simple and small molecules. Cyclic peptides are conformational restricted peptides that, thanks to their easy synthesism and complex and environment-dependent structure, are very valuable building blocks. In addition, they are also biocompatible and more stable than linear derivatives. In this regard, α-*D,L*-cyclic peptides are synthetic peptides that tend to adopt a planar conformation, predisposing them to stack and form hollow cylindrical structures.[1] The planarity of these CPs makes the linear supramolecular polymeric growth mainly driven by the backbone-backbone interations. Furthermore, this conformation darranges all the amino acid side chains so that they are oriented ouward radilly from the central cylinder. Therefore the side-chain-to-side-chain interactions provide a way for further growth, forming other type of structures as fibers, hydrogels, and 2D and 3D materials.[2] In this communication we will evaluate the approaches for developing different types of hierarchical suporamolecular organizations for precise control.[3]



REFERENCES

1. Ghadiri, M. R.; Granja, J. R.; Milligan, R. A.; McRee, D. E.; Khazanovich, N. *Nature* **1993**, *366*, 324.
2. J. R. Granja, et al. *Angew. Chem. Int. Ed*. **2020**, *59*, 6902; Granja, J. R.; *et al. Chem* **2023**, *9*, 3365; Montenegro, J.; *et al. Chem. Sci*. **2023**, *14*, 14074.
3. Granja, J. R. et al. *Angew. Chem. Int. Ed.* **2025,** e14543.

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P450 Compound I: Is it really a blowtorch?

Michael T. Green

Department of Chemistry, University of California, Irvine
Department of Molecular Biology and Biochemistry, University of California, Irvine

Much of our current understanding of metal–oxo–mediated C–H bond activation is rooted in ground-state thermodynamics, often manifested as linear free-energy relationships (LFERs). Within this framework, metal–oxo reactivity toward C–H bonds is governed by D(O–H), the strength of the O–H bond formed during hydrogen-atom abstraction. It has become clear, however, that not all systems display LFER behavior, motivating consideration of additional factors such as oxo spin density, metal–oxo basicity, and access to low-lying excited states. Cytochrome P450 is widely regarded as a biological "blowtorch": its active intermediate, P450 compound I, is capable of cleaving unactivated C–H bonds with rate constants on the order of 10^7 M^{-1} s^{-1}. Given this, remarkably little is known about the thermodynamic driving force for C–H bond cleavage by P450s or the factors that affect this reactivity. In particular, the O–H bond strength of compound II, which directly reflects P450's contribution to the driving force for hydrogen-atom abstraction, has not been experimentally determined. Here, we report our efforts to determine this quantity.

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Plant virus-corrole hybrids as bio-inspired antiviral nanomaterials

Claude P. Gros,[a] Shivani Kessavdjee-Djouma,[a,b] Nicolas Desbois,[a] Haziq Naseer Khan,[b] Tomas Moravec,[c] Nguyet-Thanh Ha Duong[b]

[a] *Université Bourgogne Europe, ICMUB - UMR CNRS 6302, 21000 DIJON France*
[b] *Université Paris Cité, ITODYS (UMR CNRS 7086),75205 Paris Cedex 13, France*
[c] *Institute of Experimental Botany, Prague 6, 16502, Czech Republic*

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The development of orthopoxvirus countermeasures is by now a top priority for health agencies, as new strains are emerging and spreading rapidly within the population. This is particularly true of the MPXV, which was responsible for the 2025 Mpox outbreak, that infected over 38,000 people [1]. We synthesized fluorocorrole derivatives, functionalized with reactive groups, and encapsulated them in Tobacco mosaic virus (TMV). The resulting nanoconjugates have a high loading capacity and demonstrate enhanced in vitro antiviral activity against the vaccinia virus compared to uncapsulated corroles. The present study establishes plant virus-corrole hybrids as a new class of bio-inspired antiviral nanomaterials for the first time [2]. Significantly enhanced antiviral activity against the vaccinia virus, a model for MPXV, was achieved by successfully encapsulating fluorocorrole derivatives within the robust and biocompatible TMV capsid. Thus, these results emphasize the versatility of TMV as a high-capacity, tunable delivery platform. Interestingly, the corrole-TMV assemblies described in this study could lead to the further development of stable, targeted antiviral nanotherapeutics.

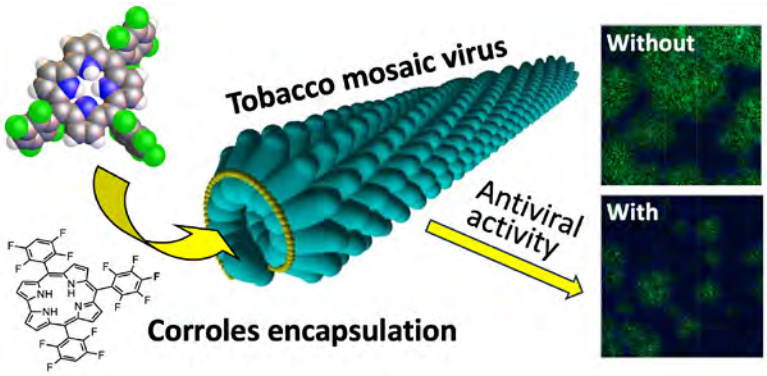


Figure 1

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REFERENCES

1. https://worldhealthorg.shinyapps.io/mpx_global/#3_Global_situation_update
2. S. Kessavdjee-Djouma, T. Moravec, H. N. Khan, S. Kappler-Gratias, F. Gallardo, N. Desbois, N.-T.-H. Duong and C. P. Gros, Plant virus-corrole hybrids as bio-inspired antiviral nanomaterials, submitted.

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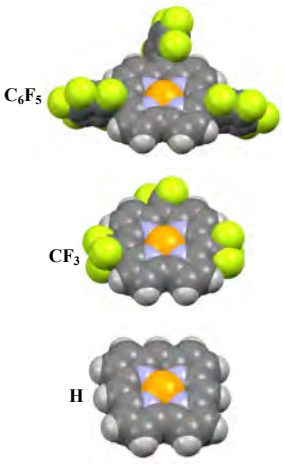


Minimally Substituted Corroles for Testing Structural and Electronic Effects on Fundamental Properties and Electrocatalysis

Zeev Gross

Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, Haifa 32,000, Israel

Almost 50 years of focus on octaalkylated corrole were replaced by 25 years of intense research on the much more accessible triarylcorroles,[1] followed by most recent advances in the synthesis of derivatives that have either no (i.e., the parent corrole) or only C1 substituents.[2-4] Armed by corroles that differ so much in terms of electron-withdrawing capability (e.g., CF_3 > C_6F_5 >> H) and size (e.g., C_6F_5 >> CF_3 >> H) paves the way for research that focuses on both fundamental and practical aspects. This presumption is actively been tested by exploring quite different aspects that include the following examples: a) the effect of axial ligands coordinated to the cobalt(III) complexes of the parent corrole on ^{1}H NMR spectra and if or how this relates to aromaticity; new insights into what determines the planarity of the corrole macrocycle and the relative orientation of ligands in 6-coordinate metal complexes; and differences in efficacy, selectivity and even reaction mechanism when used as electrocatalysts under both homogeneous and heterogenous (metallocorrole-modified electrodes) conditions.[5-8]



REFERENCES

1. A. Mahammed, H.B. Gray and Z. Gross “Silver Anniversary of the Renaissance in Metallocorrole Chemistry”, *Chem. Rev*. **2025**, *125*, 2809−2845.
2. A. Kumar, P. Yadav, M. Majdoub, I. Saltsman, N. Fridman, S. Kumar, A. Kumar, A. Mahammed and Z. Gross “Corroles: The Hitherto Elusive Parent Macrocycle and its Metal Complexes” *Angew. Chem.* **2021**, *60*, 25097-25103.
3. A. Raslin, Z. Sercel, N. Fridman, I. Saltsman and Z. Gross “The Surprising Route to a Monoazaporphyrin and Full Characterization of its Complexes with Five Different 3d Metals”, *Inorg. Chem.* **2024**, *63*, 7828–7837.
4. A. Saini, N. Fridman, A. Mahammed and Z. Gross “Triscyanocorrole, the Newest and Most Intriguing Member of the C1-Substituted Corrole Family”, *Chem. Eur. J.* **2024**, e202403642.
5. A. Raslin, J. Douglin, A. Kumar, M. Fernandez-Dela-Mora, D. Dekel and Z. Gross “Size and electronic effects on the performance of (corrolato)cobalt-modified electrodes for ORR catalysis”. *Inorg. Chem.* **2023**, *62*, 14147–14151.
6. A. Kumar, S. Fite, A. Raslin, S. Kumar, A. Mizrahi, A. Mahammed, and Z. Gross “Beneficial Effects on the Cobalt-Catalyzed Hydrogen Evolution Reaction Induced by Corrole Chelation”. *ACS Catal.* **2023**, *13*, 13344-13353.
7. S. Kumar, A. Raslin, S. Mondal, A. Mizrahi, N. Fridman, A. Mahammed and Z. Gross “Peripheral Bromination for Strongly Affecting the Structural, Electronic, and Catalytic Properties of Cobalt Corroles”, *Inorg. Chem*. **2025**, *64*, 11069−11074.
8. S. Kumar, S. Fernández, I. Saltsman, N. Fridman, A. Mahammed, A. J. M. Miller and Z. Gross “Substituents Effects on the Electrocatalytic CO_2 Reduction by Cobalt Corroles in Solution”, *Chem. Commun*. **2025**, *61*, 12924 – 12927.

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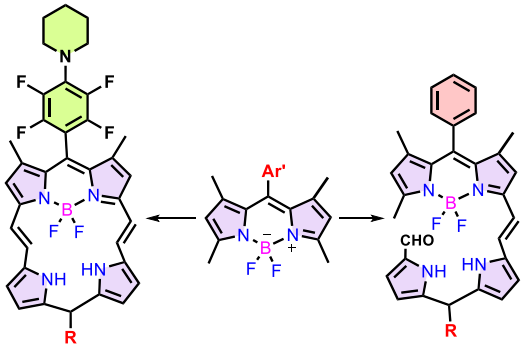
Synthesis and Photophysical Analysis of BODIPY-DPM Conjugates

Nitika Grover

Department of Chemistry, BITS Pilani Pilani Campus, Rajasthan -333031, India
Email: nitika.grover@pilani.bits-pilani.ac.in

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Organic dyes with tunable electronic and optical properties are becoming an important tool in modern biomedicine, imaging, and phototherapies. Among these, boron dipyrromethenes (BODIPYs) gained special attention due to their modular design, strong absorption, and low toxicity, making them excellent photosensitizers (PSs) for photodynamic therapy (PDT).[1] Traditional triplet harvesting via heavy atoms enhances intersystem crossing (ISC) but compromises biocompatibility and stability. Consequently, recent efforts emphasize heavy-atom-free molecular designs that achieve efficient ISC through structural engineering, such as BODIPY–anthracene and benzothiophene-fused systems with enhanced spin–orbital coupling and strong ROS generation.[2,3] Parallel studies on dipyrrin and dipyrromethane (DPM) derivatives, including prodigiosin analogues, reveal potent anticancer and antimicrobial properties, underscoring the biomedical potential of pyrrole-based scaffolds. Inspired by these advances, we envisioned merging BODIPY with dipyrrin/DPM frameworks to create multifunctional, heavy-atom-free systems integrating imaging, anticancer, and antimicrobial capabilities. We selected 5-tolyl-1,3,7,9-tetramethyl BODIPY as a model substrate. Reaction with pyrrole-2-carboxaldehyde under microwave irradiation yielded the mono- and di-substituted derivatives depending on aldehyde stoichiometry. Extending this, condensation of BODIPY with various DPMs furnished mono- and cyclic BODIPY–DPM conjugates in good yields. Further, we tested the $^1O_2$ generation capabilities of synthesized compounds. These results demonstrate a versatile strategy for constructing BODIPY–DPM hybrids, uniting efficient triplet harvesting with potential biomedical functionality in next-generation photosensitizers.



REFERENCES

1. I S Yadav and R. Misra *J. Mater. Chem. C*, **2023**,*11*, 8688.
2. W Bu, C Yu, Y Man, J Li, Q Wu, S Gui, Y Wei, L Jiao and E. Hao *Chem. Commun.*, **2024**, *60*, 9809.
3. M A Filatov, S Karuthedath, P M Polestshuk, H Savoie, K J Flanagan, C Sy, E Sitte, M Telitchko, F Laquai, R W Boyle, M O Senge *J. Am. Chem. Soc* **2017**, *139*, 6282.

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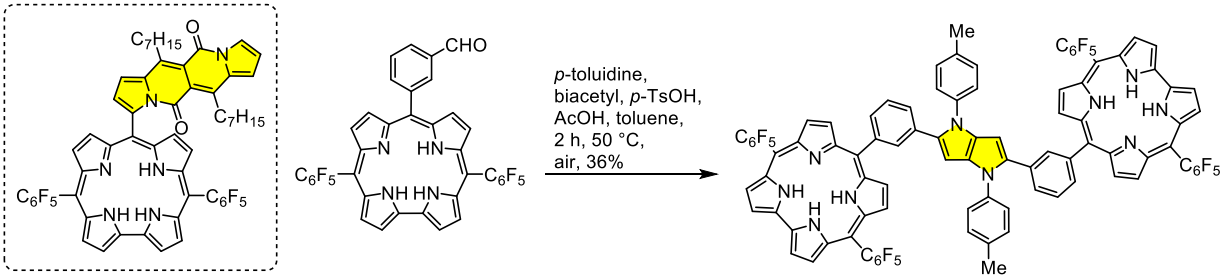
Novel π-expanded corroles

Daniel T. Gryko[a], **Beata Koszarna**,[a] **Łukasz Kielesiński**[a]

[a]*Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland*

In 1998, it would have been impossible to imagine that only 25 years later the chemistry of corroles would expand to create an independent field of study. The synthesis of *meso*-substituted corroles evolved quickly during the first seven years after Paolesse's and Gross's discovery [1,2,3]. Although the synthetic revolution made it possible to try risky ideas in diverse areas of materials chemistry and in various biology- and medicine-oriented applications, multiple challenges still remain.

Traditionally π-expansion of given chromophore is realized *via* fusion with another aromatic unit. Given however that in some cases an electronic communication *via* biaryl linkage is very strong, bridging corrole with other heterocycles represents an alternative strategy. Herein we will present a few approaches leading to meso-substituted corroles linked with e.g. 1,4-dihydropyrrolo[3,2-*b*]pyrrole and dipyrrolonaphthyridinedione. The photophysical properties of the resulting *trans*-A_2B-corroles are intriguing. We discovered that the 10-(3-formylphenyl)corrole can be used in the synthesis of 1,4-dihydropyrrolo[3,2-*b*]pyrrole bearing two corrole macrocycles. The multicomponent reaction heavily depends in this case on position of the formyl group. We also found that in spite of large dihedral angle the presence of various π-systems at positions 5 and 10 of corrole core leads to substantial changes in the photophysical properties.



REFERENCES

1. Gross, Z.; Galili, N.; Saltsman, I. *Angew. Chem. Int. Ed.* **1999**, *38*, 1427−1429.
2. Paolesse, R.; Jaquinod, L.; Nurco, D. J.; Mini, S.; Sagone, F.; Boschi, T.; Smith, K. M. *Chem. Commun.* **1999**, 1307−1308.
3. Koszarna, B.; Gryko, D. T. *J. Org. Chem*. **2006**, *71*, 3707−3717.

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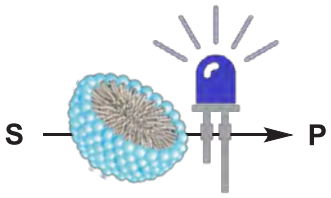
Photochemical reactions in aqueous micellar environment

Dorota Gryko[a]

[a]*Institute of Organic Chemistry Polish Academy of Sciences, Kasprzaka 44/52, 01p-224 Warsaw, Poland*

ORALS

Bioinspiration is a well-established approach in the field of chemistry. Although in biological systems reactions take place in water-based confined compartments, organic chemists have for a long time, assumed that water is not a suitable medium for reactions of lipophilic reactants. Micellar solutions do, however, allow their incorporation into the confined system, thus fostering their reactions.[1] Although pioneering contributions have shown that harnessing aqueous media for organic synthesis may bring various benefits, ranging from reduced environmental impact, increased reactivity, milder reaction conditions, improved chemo, regio, and stereoselectivity, to safer reaction conditions, these systems, however, are not widely utilized in synthetic organic chemistry, even less so for reactions involving radicals.[1b,c]



Along this line, we have demonstrated that visible light-driven reactions can be conducted in aqueous environments. For example, cobalt-catalyzed radical addition/1,2- aryl migration,[2] epoxide ring opening,[3] cyclopropanation with diazo compounds,[4] and CO_2 cycloadditions[5] afforded the desired products in high yields and selectivity. A series of NMR measurements and theoretical studies revealed the location of reaction components in the micellar systems. Our work expands the chemical space related to both photocatalysis and the aqueous micellar environment, opening access to a new research area at the intersection of photocatalysis and biocatalysis fields.

REFERENCES

[1] Cortes-Clerget, M.; Yu, J.; Kincaid, J. R. A.; Walde, P.; Gallou, F.; Lipshutz, B. H. *Chem. Sci.* **2021**, *12*, 4237. (b) Brüss, L.; Jeyaseelan, R.; Kürschner, J. C. G.; Utikal, M.; Næsborg, L. *ChemCatChem* **2023**, *15*, 9. (c) Russo, C.; Brunelli, F.; Tron, G. C.; Giustiniano, M. *J. Org. Chem.* **2022**. *88*, 6284.

[2] Wincenciuk, A.; Cmoch, P.; Giedyk, M.; Andersson, M. P.; Gryko, D. *J. Am. Chem. Soc.* **2024**, *146*, 19828.

[3] Szabó, K. F.; Wdowik, T.; Krzeszewska, A.; Mazurek, K.; Andersson, M. P.; Gryko, D. *Org. Lett.* **2025**, *27*, 5642.

[4] Milton, J. P.; Milanowski, A.; Andersson, M.; Gryko, D. *Chem. Commun.*, **2024**,60, 4483.

[5] Depa, W. ; Majumder, S. ; Nadirowa, M. ; Cmoch, P. ; Andersson, M. P.; Gryko, D. *Chem Catal*. **2026**, accepted

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Exciton Migration in Porphrinic Systems

Dirk M. Guldi[a]

[a]*Friedrich-Alexander-Universität Erlangen-Nürnberg FAU Profile Center Solar Department of Chemistry and Pharmacy Interdisciplinary Center for Molecular Materials (ICMM) Egerlandstr. 3, 91058 Erlangen*

Light-induced intramolecular charge transfer and energy transfer processes on the nanoscale are effectively modulated through rational molecular design, particularly by architectures incorporating electron and/or energy donor-acceptor motifs. Of utmost importance is exciton migration, the movement of excitation energy away from its site of generation. This process is often mediated by interactions between molecular building blocks through Förster resonance energy transfer. Motivated by the above considerations, we have undertaken a deeper inquiry into designing anthryl-ethynyl-aniline / anthryl-aniline building blocks coupled to zinc porphyrins at their meso-positions. Importantly, the ethynyl bridge is known to modulate the triplet energy levels of anthracene, while the amine group serves as a strong electron donor. In this scenario, several metastable excited states with comparable energies arise as a result of the nearly orthogonal arrangement of the chromophoric units. Our results demonstrate exciton migration on the ultra-long timescale due to a dynamic equilibrium between two localized triplet excited states. The key is the mixing of two localized triplet excited states with a delocalized exciton state, independent of photoexcitation wavelength and solvents.

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Exploring Photocatalysis with Metal Dipyrrinato Complexes

Iti Gupta*[a], Kritika Agarwal, Samrita Sharma

[a]*Department of Chemistry, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar-382355, Gujarat, India. E-mail: iti@iitgn.ac.in*

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Visible-light photocatalysis is an environmentally benign method for driving complex chemical transformations, particularly oxidation processes [1]. The field of photoredox catalysis has been revolutionized by Ru(II) and Ir(III) organometallic complexes, with the benchmark catalyst *fac-Ir (ppy)*$_3$ (ppy = 2-phenylpyridine) widely adopted in synthetic organic transformations. In general, Ru(II) and Ir(III) polypyridyl complexes and organic dyes have been used for photocatalyzed organic transformations [2]. The heteroleptic complexes of Pd(II), Re(I), and Ir(III) with a dipyrrin ligand have been found to be excellent photocatalysts for the oxidation of organic molecules [3, 4]. Their attractive photophysical properties and long-lived triplet states boost the production of reactive oxygen species and singlet oxygen, which is very helpful for oxidation processes.

The work focuses on the synthesis and characterization of a series of heteroleptic Ir(III) and Re(I) dipyrrinato complexes [5]. We will demonstrate a synthetic protocol for the photocatalyst-mediated oxidation of indole derivatives, sulfoxidation and benzyl amine coupling reaction under blue light and/or sunlight. The results of DFT calculations will also be discussed to explain the reaction mechanism of selected reactions.

REFERENCES

[1] Janaagal, A.; Sanyam; Mondal, A.; Gupta, I. J. Org. Chem. 2023, 88, 9424-9431.
[2] Shaw, M. H.; Twilton, J.; MacMillan, D. W. C. J. Org. Chem. 2016, 81, 6898−6926.
[3] Kumar, S.; Devi, L.; Gupta, I., New J. Chem., 2025, 49, 11080-11088.
[4] Kumar, S.; Agarwal, K.; Sanyam; Mondal, A.; Gupta, I. Chem. Asian J., 2024, e202400680.
[5] Devi, L.; Sharma, S.; Agarwal, K.; Gupta, I. Appl. Organomet. Chem., 2025, 39, e70427.

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Applications of small angle scattering to delineate P450-membrane and redox partner interactions.

John C Hackett, Kamila Stokowa-Sołtys, and Francisco Zarate-Perez

Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199 U.S.A

Small-angle X-ray and neutron scattering (SAX/NS) are potent tools for elucidating the structures of biological macromolecules and their complexes. Although resolution is comparatively low compared to methods such as crystallography, electron microscopy, and NMR, SAX/NS offers the advantage of obtaining structural information from readily prepared, small samples without molecular size limitations. When combined with contemporary structure prediction tools and molecular dynamics simulations, SAX/NS becomes an invaluable instrument for investigating conformational ensembles of flexible molecules and the architectures of macromolecular complexes. In this presentation, I will describe the applications of SAX/NS and molecular simulation to pertinent cytochromes P450 and their redox partner interactions. Initially, I will describe how contrast variation SANS was integrated with a molecular dynamics flexible fitting approach to delineate the orientation and interactions of cytochrome P450 reductase with lipoprotein nanodiscs. Subsequently, I will present how SAXS, coupled with size exclusion chromatography, was employed in conjunction with artificial intelligence-based structural predictions and molecular dynamics simulations to derive a novel atomistic model of the interaction between CYP17A1 and cytochrome b_5. I anticipate that these case studies will underscore the utility of combining small angle scattering with contemporary computational methods to advance our comprehension of membrane and redox partner interactions within P450 systems.

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Ultrafast Molecular Spin Coherence for Quantum Transduction in Complex Environments

Ryan G. Hadt[a]

[a]*Division of Chemistry and Chemical Engineering, Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125, United States*

Molecular electron spins offer a uniquely tunable platform for quantum science, linking quantum coherence to chemical structure and environment. In this talk, I will describe how ultrafast, all-optical measurements enable direct observation of molecular spin coherence under ambient conditions. By using light to both prepare and read out spin states, these approaches reveal how molecular motion, local interactions, and surrounding media influence quantum coherence in real time. I will highlight how spin coherence can act as a sensitive probe of molecular dynamics and chemical environments and discuss emerging opportunities for using molecular spins as quantum tranducers that bridge photons, spins, and complex chemical and biological systems. Together, these results point toward new strategies for molecular-level quantum sensing and imaging based on ultrafast spin coherence.

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The Two Faces of Photoimmunotherapy

Tayyaba Hasan

[a]*The Wellman Center for Photomedicine, Massachusetts General Hospital and Harvard Medical School, Boston, MA 02114; Division of Health Sciences and Technology, Harvard University and Massachusetts Institute of Technology, Cambridge, MA 02139*

Photoimmunotherapy (PIT) can come in many flavors. One in which the immune agent, such as antibodies, polymers, or peptides, is used to deliver photosensitizers. The major attribute of this form of PIT is that an immune agent with varying specificity is used primarily as a delivery vehicle, although its inherent immunogenicity will help induce an immune response. So, this form of PIT has both specific targeting and immunogenicity. In addition, targeting can be multiple-fold with Bispecific antibodies or serve dual functions, providing both targeted killing and multimodal imaging capabilities.

The second PIT form, which we call Neoadjuvant PIT or NAPIT, is performed prior to an immune agent, such as immune checkpoint inhibitors (ICIs). The photodynamic activation primes the tumor tissue, a process we term photodynamic priming (PDP) that alters the microenvironment. The PDP provides enhanced permeability, allowing immune cells to enter tumor tissues, which is particularly significant in more stromal cell-dominated tumors such as Pancreatic ductal adenocarcinoma (PDAC). As immune cells interact with tumor cells, the PDP also initiates cytokine and other responses that have remote effects on the cellular niche, away from the primary tumors. This results in decreasing or abrogating metastases.

Both of these forms of photoimmunotherapy are important to explore, and I will discuss results from our laboratory on both of these faces.

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Single Crystal Field-Effect Transistor of Tetrabenzoporphyrin with a One-Dimensional Columnar Packing Motif

Hironobu Hayashi[a], **Hiroko Yamada**

[a]*Center for Basic Research on Materials, National Institute for Materials Science (NIMS)*
[b]*Institute for Chemical Research (ICR), Kyoto University*

ORALS

Tetrabenzoporphyrins (BPs) possess large, rigid, and planar π-conjugated systems, making them promising candidates for efficient p-type organic semiconductors due to their potential for strong π–π orbital overlap facilitating charge transport. However, their poor solubility in common organic solvents has limited solution-processable device fabrication. To overcome this, the introduction of triisopropylsilyl (TIPS) ethynyl groups improves solubility and enables solution processing. Here, 5,15-bis(triisopropylsilyl-ethynyl)tetrabenzoporphyrin (TIPS-H_2BP) exhibits sufficient solubility and forms distinct molecular packing motifs, including a one-dimensionally extended columnar structure favorable for charge transport. In this study, single crystals of TIPS-H_2BP and its zinc and copper metal complexes were grown on octadecyltrichlorosilane-modified Si/SiO_2 substrates via slow drop-casting. Structural characterization by single-crystal X-ray diffraction and transmission electron microscopy revealed that TIPS-H_2BP molecules stack in a well-ordered, one-dimensional columnar motif with a π–π stacking distance of approximately 3.3 Å. This contrasts with the triad-like packing observed in the metal complexes, which lack long-range molecular orientation. Organic field-effect transistors fabricated using these single crystals demonstrated that TIPS-H_2BP achieved a maximum hole mobility of 2.16 $cm^2\ V^{-1}\ s^{-1}$. The enhanced mobility is attributed to the high crystallinity and favorable molecular orientation enabling efficient charge transport along the π-stacked columns. Conversely, the metal complexes exhibited significantly lower mobilities (~0.1 $cm^2\ V^{-1}\ s^{-1}$) due to their less ordered triad packing, which hinders charge transport.[1]

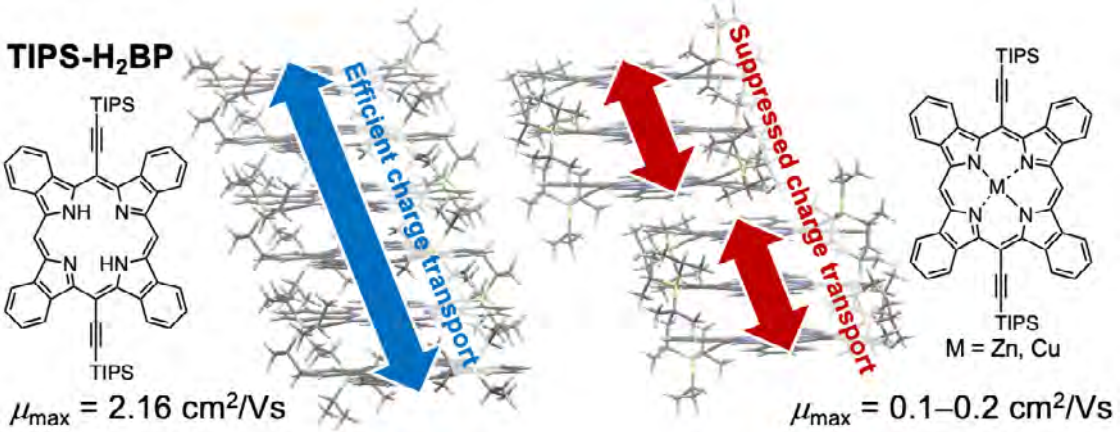


Figure 1. Packing structures and hole mobilities of TIPS-H_2BP and its metal complexes.

REFERENCES

1. J. Zhu, H. Hayashi, M. Chen, C. Xiao, K. Matsuo, N. Aratani, L. Zhang, H. Yamada, *J. Mater. Chem. C* **2022**, *10*, 2527.

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Switchable Systems Incorporating Porphyrins

Valérie Heitz

Laboratoire de Synthèse des Assemblages Moléculaires Multifonctionnels, Institut de Chimie de Strasbourg, CNRS/UMR 7177, Université de Strasbourg, E-mail: v.heitz@unistra.fr

Porphyrins have been widely integrated into covalent and supramolecular systems owing to their remarkable coordination abilities and their attractive electronic and photophysical properties. The synthesis of receptors incorporating metalloporphyrins as active elements has led to highly appealing architectures for molecular recognition and chemical transformation. The introduction of chemical, redox, or photoresponsive units further enables precise control over the properties of porphyrin-based hosts, including guest uptake, catalysis, and drug transport.[1] Our group has designed a variety of porphyrin-containing receptors, such as cages and tweezers, that include triazole[2], or acridinium[3] as responsive units. This presentation will discuss the design, optical properties, and responsiveness of some representative systems to different stimuli (chemical, electronic, and photonic).

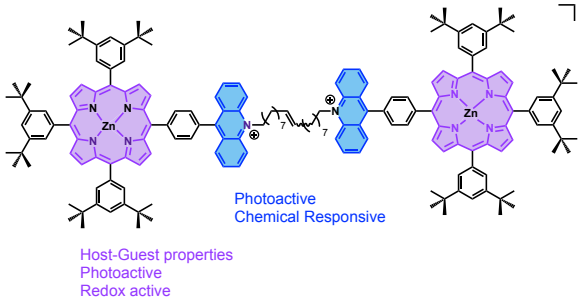


Fig. Exemple of a tweezer incorporating two stimuli-responsive units.

REFERENCES

1. S. Durot, J. Taesch, V. Heitz, *Chem. Rev.* **2014**, *114*, 8542; A. J. McConnell, C. S. Wood, P. P. Neelakandan, J. R. Nitschke, *Chem. Rev.* ***2015****, 115,* 7729; A. Blanco-Gómez, P. Cortón, L. Barravecchia, I. Neira, E. Pazos, C. Peinador, M. D. García, *Chem. Soc. Rev.* **2020**, *49*, 3834–3862.
2. R. Djemili, L. Kocher, S. Durot, A. Peuronen, K. Rissanen, V. Heitz, *Chem. Eur. J.* **2019**, *25*, 1481; L. Zanetti-Polzi, R. Djemili, S. Durot, V. Heitz, I. Daidone, B. Ventura, *Chem. Eur. J.* **2020**, *26*, 17514; L. Schoepff, L. Monnereau, S. Durot, S. Jenni, C. Gourlaouen, V. Heitz, *ChemCatChem* **2020**,*12*, 5826; R. Djemili, S. Adrouche, S. Durot, V. Heitz, *J. Org. Chem.* **2023**, *88*, 14760.
3. Edo-Osagie, D. Serillon, F. Ruani, X. Barril, C. Gourlaouen, N. Armaroli, B. Ventura, H.-P. Jacquot de Rouville, V. Heitz *J. Am. Chem. Soc.* **2023***, 145,* 10691–10699. F. Ruani, D. Veclani, D. Sanchez-Resa, A.Edo-Osagie, G. Creste, A. Barbieri, V. Heitz, H.-P. Jacquot de Rouville, N. Armaroli, B. Ventura, *Chem. Eur. J.*, **2025**, e02604.

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Role of the CuB Center in the Formation and Stabilization of the F-State in Cytochrome *c* Oxidase from *Paracoccus denitrificans*

Petra Hellwig[a*], Raaif Siddeeque[a], Daniel Hatlem[b], Hartmut Michel[b], Frédéric Melin[a]

[a] *Laboratoire de Bioélectrochimie et Spectroscopie, UMR 7140, Chimie de la Matière Complexe, Université de Strasbourg – CNRS 4, rue Blaise Pascal, 67081 Strasbourg, France * hellwig@unistra.fr*
[b] *Department of Molecular Membrane Biology, Max Planck Institute of Biophysics, Max-von-Laue-Str. 3, D-60438 Frankfurt/Main, Germany*

The selective four-electron reduction of molecular oxygen to water is a fundamental biological process catalyzed by terminal oxidases in aerobic organisms. Despite extensive structural information on cytochrome c oxidases, key aspects of their molecular mechanisms—particularly in bacterial systems—remain unresolved. In this study, the catalytic cycle of oxygen reduction in *Paracoccus* cytochrome c oxidase was investigated in the presence of hydrogen peroxide (H_2O_2) using UV–visible absorption spectroscopy and resonance Raman spectroscopy. Both native (ATCC) and recombinant enzyme forms were analyzed. Comparative evaluation against existing mechanistic models revealed strain-dependent variations in the reaction pathway, supporting and extending previous interpretations.

Special emphasis was placed on the role of the copper B (CuB) center within the binuclear catalytic site. Spectroscopic data indicate that the intermediate previously assigned as the F-state corresponds to a superoxide-bound species coordinated to CuB rather than to the heme iron. This reassignment prompted a revised view of electron transfer and intermediate stabilization during oxygen reduction, highlighting an active role for CuB. Isotopic labeling experiments using ^{65}Cu- and ^{63}Cu-enriched enzymes, combined with resonance Raman analysis, enabled direct identification of copper coordination in this catalytic intermediate. Furthermore, two CuB-deficient variants (H276K and H276D) were examined to assess the functional significance of this site. Structural and spectroscopic characterization demonstrated that loss of CuB impairs formation and stabilization of the F-state, underscoring its critical contribution to efficient oxygen reduction.

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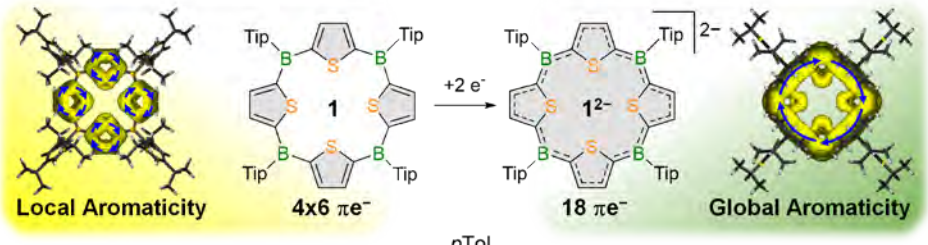


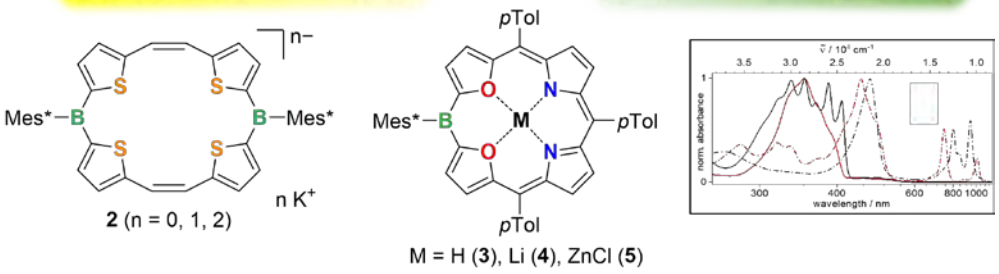
Boron-Doped Porphyrinoids: Combining Lewis Acidity with Redox-Switchable Aromaticity

Holger Helten*[a]

[a]*Julius-Maximilians-Universität Würzburg, Institute of Inorganic Chemistry and Institute for Sustainable Chemistry & Catalysis with Boron (ICB), Am Hubland, 97074 Würzburg, Germany.*

The structural motif of porphyrin – ubiquitous in living nature and relevant for various essential biological processes – has evolved into a highly versatile building block of functional materials. Incorporation of trivalent boron via its vacant p_π orbital in an organic π system can generate unique properties and functions. We combine both features by doping the macrocyclic framework of porphyrin and related macrocycles with electron-deficient boron centers. We recently developed tetrathiaporphyrinogen **1** having boron atoms in all four *meso*-positions [1]. The antiaromaticity in this macrocycle is effectively concealed by the local aromaticity confined in the constituent thiophene units. Global aromaticity is switched on by facile electrochemical or chemical reduction. The bowl-shaped radical anion $\mathbf{1}^{-}$ and the dianion $\mathbf{1}^{2-}$ exhibit absorption features that are typical of porphyrins, while the latter shows significantly enhanced low-energy Q-bands. The expanded diboraporphyrinoid **2**, on the other hand, is notably antiaromatic in the neutral state and is transformed into a globally aromatic macrocycle upon reduction [2]. The 5-bora-21,22-dioxaporphyrin **3** and its main-group and d-block metal complexes **4** and **5** constitute the first examples of neutral porphyrins with boron in a *meso*-position that exhibit global aromaticity [3]. These novel macrocyclic boranes exhibit panchromatic absorption and photoluminescence in the NIR spectral region.





REFERENCES

1. Buckel, M.; Klopf, J.; Schneider, J. S.; Lik, A.; Riensch, N. A.; Krummenacher, I.; Braunschweig, H.; Engels, B.; Helten, H. *Nat. Commun.* **2025**, *16*, 1775.
2. Swoboda, L.; Klopf, J.; Buckel, M.; Engels, B.; Helten, H. *J. Am. Chem. Soc.* **2026**, *148*, DOI: 10.1021/jacs.5c18822.
3. Swoboda, L.; Klopf, J.; Fest, M.; Friedrich, A.; Buckel, M.; Krummenacher, I.; Braunschweig, H.; Engels, B.; Helten, H. *J. Am. Chem. Soc.* **2025**, *147*, 10629−10639.

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In vitro and In Cell Conversion of Prostaglandin H_2 into A Bioactive Fatty Acid Catalyzed by Cytochrome P450 Mimics

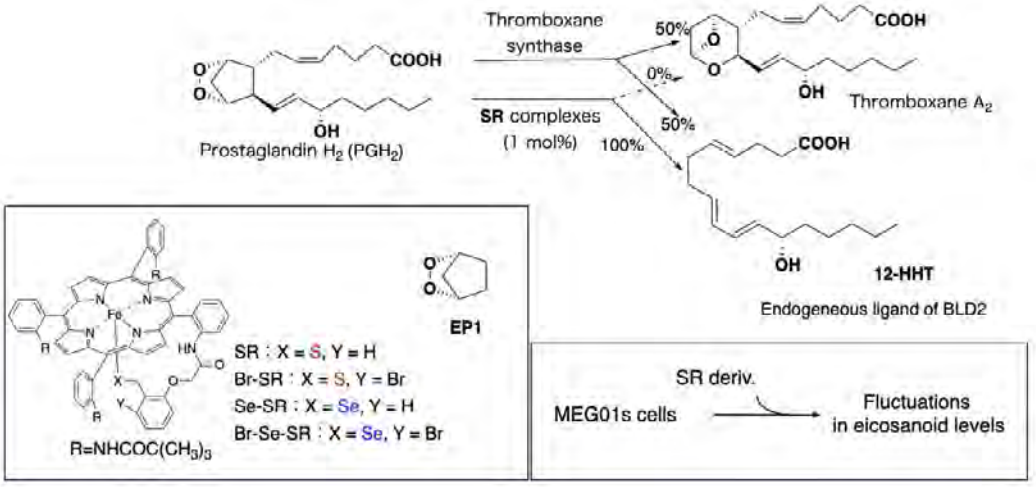
Tsunehiko Higuchi[a] , Yuto Tsuzuki[a], Yosuke Hisamatsu[a], Naoki Umezawa[a], Min Liu[b], Kazuko Saeki[b], Takehiko Yokomizo[b]

[a]*Graduate School of Pharmaceutical Sciences, Nagoya City University*

[b]*Graduate School of Medical Science, Juntendo University*

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Prostaglandins (PG) are biosynthesized by isomerizing the common intermediate PGH_2, which is a cyclic peroxide, with different enzymes. Two of the enzymes (thromboxane A_2 synthase and PGI_2 synthase) are known to be cytochrome P450 type ones. We have developed highly stable, unique **SR** complexes having a coordination structure (thiolate-coordinated heme) similar to P450.[1] **SR** complexes as P450 mimics catalyze a number of P450-like reactions with high efficiency. Previously, we reported a cyclic peroxide EP1, the head part of PGH_2, was efficiently converted into the isomerized product and split product catalyzed by **SR** complex.[2] We have also found that **SR** complex rapidly isomerized PGH_2 to form 12-HHT exclusively. Yokomizo (collaborator) and coworkers found that 12-HHT is an endogenous ligand of receptor BLT2 and has skin wound healing activity.[3] Therefore, we expected that P450 mimic such as **SR** enhances production of 12-HHT to lead skin wound healing by catalyzing PGH_2 conversion in cells. We analyzed the change of amount of each related lipid in cells by administration of 4 kinds of P450 mimics comprehensively. We found administration of 1 μM of **SR** complex to human cells increased 12-HHT level by 1.5 fold and decreased PGE_2 level which arouses pain. The results suggest that **SR** complex promote wound healing while reducing wound pain.



REFERENCES

1. T. Higuchi. S. Uzu, M. Hirobe *J. Am. Chem. Soc.*, **1990**, *112*, 7051-7053.
2. T. Yamane, K. Makino, N. Umezawa, N. Kato, T. Higuchi *Angew. Chem. Int. Ed.* **2008**, *47*, 6438-6440.
3. T. Okuno, Y. Iizuka, H. Okazaki, T. Yokomizo, R. Taguchi, T. Shimizu *J. Exp. Med*. **2008**, *205*, 759-766.

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Self-assembled Porphyrins for Advanced Applications

Jonathan P. Hill[a]

[a]*Research Center for Materials Nanoarchitectonics, National Institute for Materials Science,Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan*

Supramolecular chemistry and self-assembly methods are key to influence aggregative processes, and can be used to control the emergent properties of self-assembled organic nanomaterials. In this work, we have studied chromophore compounds with the emphasis partly on pyrazinacenes [1] (N-heteroacenes composed of linearly fused pyrazine units) but mostly on porphyrin [2] molecules. Different properties are accessed from self-assembled structures or from solutions of the materials. Self-assembled structures are obtained using Langmuir and Langmuir-Blodgett techniques, nanoparticle synthesis, and solution-based crystallization. Principles of amphiphilicity have been applied to generate on-interface structures that can be extracted as multilayered films and exploited for application in electronic devices. Here, we will describe the sensing [3], photosensitization [4] (to generate singlet oxygen), and other [5,6] properties of the materials based on molecular structure and state of aggregation. We also describe printable structures for sensing applications based on interleaved microcrystalline forms. Molecular structure is emphasized as a key feature including the effects of structural amphiphilicity, π-π stacking, and conformational flexibility. Self-assembly and supramolecular techniques stand out as the most effective methods for obtaining organic nanomaterials having the molecule-level definition of structure important for many applications including sensing and photosensitization. From this point-of-view, applications based on supramolecular effects or device incorporation of self-assembled materials will be discussed. In particular, several new classes of singlet oxygen photosensitizer have been established as well as selective sensing of vapor analytes using porous self-assembled structures.

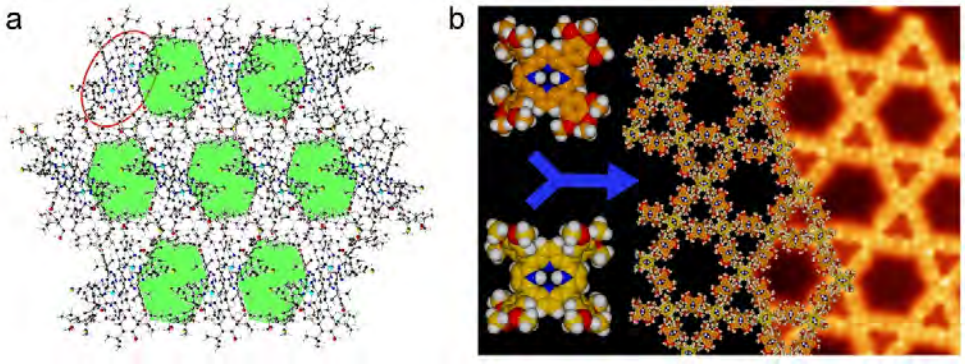


Figure. **a**, Self-assembled porous crystals of beta-substituted porphyrins. **b**, Two-dimensional porphyrin Kagome.

REFERENCES

1. G. J. Richards and J. P. Hill, *Acc. Chem. Res*., **2021**, *54*, 3228.
2. S. Maji, J. P. Hill, et al. *Adv. Mater. Technol.*, **2025,** in press.
3. M. K. Chahal, J. P. Hill, et al. *Mater. Chem. Front.*, **2023**, *7*, 325.
4. C. Bloyet, J. P. Hill, et al. *J. Am. Chem. Soc.* **2022**, *144*, 10830.
5. G. J. Richards, J. P. Hill, et al. *Angew. Chem. Int. Ed*. **2025**, *64*, e202504564.
6. D. Jiang, J. P. Hill, et al. *J. Am. Chem. Soc.* **2025**, *147*, 12460.

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Computational Studies on Cytochrome P450: Reactivity in Drug Metabolism and Bonding Characteristics of Key Intermediates

Hajime Hirao[a]

[a]*Warshel Institute for Computational Biology, School of Medicine, The Chinese University of Hong Kong, Shenzhen, Guangdong, 518172, P. R. China*

In humans, cytochrome P450 enzymes (P450s) are versatile heme-containing biocatalysts that play critical physiological and pharmacological roles. Physics-based computational approaches are expected to play a key role in elucidating the catalytic mechanisms of P450s. However, to date, relatively few studies have addressed the mechanisms involved in drug metabolism, particularly through hybrid quantum mechanics/molecular mechanics (QM/MM) calculations, highlighting the need for continued investigation. In recent years, our group has actively taken on this challenge by studying P450-catalyzed transformations of structurally complex drug molecules in the context of drug metabolism and P450 inhibition. Furthermore, we are exploring the fundamental aspects of P450 catalysis, investigating the bonding characteristics of key intermediates as well as heme–inhibitor complexes using a range of theoretical approaches, including energy decomposition analysis (EDA) and valence bond (VB) theory. In this presentation, I will discuss our recent findings in these areas.

REFERENCES

1. Hirao, H.; Yue, D.; Xia, S.; Zhang, E.; Zhang, H.; Yan, J.; Xiao, Z. Computational Studies on Human Cytochrome P450: Advancing Insights into Drug Metabolism. *Trends Chem.* **2025**, *7* (7), 358–371.
2. Yue, D.; Hirao, H. Mechanism of Selective Aromatic Hydroxylation in the Metabolic Transformation of Paclitaxel Catalyzed by Human CYP3A4. *J. Chem. Inf. Model.* **2023**, *63* (24), 7826–7836.
3. Yue, D.; Ng, E. W. H.; Hirao, H. Hydrogen-Bond-Assisted Catalysis: Hydroxylation of Paclitaxel by Human CYP2C8. *J. Am. Chem. Soc.* **2024**, *146* (44), 30117–30125.
4. Liu, S.; Xia, S.; Yue, D.; Sun, H.; Hirao, H. The Bonding Nature of Fe–CO Complexes in Heme Proteins. *Inorg. Chem.* **2022**, *61* (44), 17494–17504.
5. Hirao, H.; Zhang, E. Bidirectional Charge Transfer at the Heme Iron in Reversible and Quasi-Irreversible Cytochrome P450 Inhibition. *Inorg. Chem.* **2023**, *62* (40), 16599–16608.
6. Zhang, E.; Hirao, H. Synergistic Charge Transfer Effect in Ferrous Heme–CO Bonding within Cytochrome P450. Molecules **2024**, *29* (4), 873.
7. Zhang, E.; Hirao, H. Exploring the Bonding Nature of Iron(IV)-Oxo Species through Valence Bond Calculations and Electron Density Analysis. *J. Phys. Chem. A* **2024**, *128* (34), 7167–7176.

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Chemical tools for fluorescence imaging of labile heme in living cells and tissues

Tasuku Hirayama[a]

[a]*Laboratory of Chemical Biology, Gifu Pharamaceutical University*

Heme, a complex of protoporphyrin IX and iron, is an essential cofactor for hemoproteins such as hemoglobin, cytochrome P450, and catalase. While most heme is tightly bound to proteins and biologically sequestered, a small fraction exists as "labile heme"—a protein-free or weakly bound ferrous form that plays critical roles in cell signaling and oxidative stress [1,2]. Despite its physiological and pathological importance, the spatiotemporal dynamics of intracellular labile heme remain poorly understood. Although various fluorescent probes have been developed, improvements in sensitivity, selectivity, and usability are still required.

We have developed a series of chemical probes for labile heme based on *N*-oxide chemistry, utilizing N-oxides as ferrous-selective chemical switches. By optimizing the *N*-oxide moiety and fluorescent scaffold, we identified H-FluNox—comprising a difluoropiperidine *N*-oxide and a rhodol dye—which exhibits superior selectivity and sensitivity for labile heme. H-FluNox enabled real-time imaging of heme biosynthesis, nitric oxide-induced heme release, and heme accumulation during ferroptosis [4].

Furthermore, we expanded this *N*-oxide chemistry to tissue imaging. We found that the reaction between *N*-oxide and labile heme generates high-valent iron-oxo species, which can be trapped by electron-rich aromatics to form reactive electrophiles. This sequential reaction was utilized for a heme-activated biomolecule labeling strategy, achieving successful fluorescence imaging of heme in the mouse brain [5]. In this presentation, I will discuss the molecular design, mechanistic insights, and recent progress of our heme-imaging technologies.

REFERENCES

1. Shimizu, T.; Lengalova, A.; MartÍnek, V.; MartÍnková, M. Heme: Emergent Roles of Heme in Signal Transduction, Functional Regulation and as Catalytic Centres. *Chem. Soc. Rev.* **2019**, 48 (24), 5624－5657
2. Vasconcellos, L. R. C.; Dutra, F. F.; Siqueira, M. S.; Paula-Neto, H. A.; Dahan, J.; Kiarely, E.; Carneiro, L. A. M.; Bozza, M. T.; Travassos, L. H. Protein Aggregation as a Cellular Response to Oxidative Stress Induced by Heme and Iron. *Proc. Natl. Acad. Sci. U. S. A.* **2016**, 113 (47), No. E7474−E7482.
3. Dunaway, L. S.; Loeb, S. A.; Petrillo, S.; Tolosano, E.; Isakson, B. E. Heme Metabolism in Nonerythroid Cells. *J. Biol. Chem.* **2024**, 300 (4), 107132.
4. Kawai, K.; Hirayama, T.; Imai, H.; Murakami, T.; Inden, M.; Hozumi, I.; Nagasawa, H. Molecular Imaging of Labile Heme in Living Cells Using a Small Molecule Fluorescent Probe. *J. Am. Chem. Soc.* **2022**, *144* (9), 3793–3803.
5. Kawai, K.; Hirayama, T.; Imai, H.; Murakami, T.; Inden, M.; Hozumi, I.; Nagasawa, H. Molecular Imaging of Labile Heme in Living Cells Using a Small Molecule Fluorescent Probe. *J. Am. Chem. Soc.* **2022**, *144* (9), 3793–3803.

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Precursor State of 3D Domain Swapping in the Folding Process of Cytochrome *c*

Shun Hirota[a,b], Cheng Xie[a], Takahiro Sakai[a], Hongxu Yang[a], Tsuyoshi Mashima[a,b], Kassandra Boshae[c], Bruce Bowler[c,d], Hideaki Ogata[e]

[a]*Division of Materials Science, Graduate School of Science and Technology, Nara Institute of Science and Technology (NAIST), 8916-5 Takayama, Ikoma, Nara 630-0192, Japan*
[b]*Medilux Center, Graduate School of Science and Technology, Nara Institute of Science and Technology (NAIST), 8916-5 Takayama, Ikoma, Nara 630-0192, Japan*
[c]*Department of Chemistry & Biochemistry, University of Montana, Missoula, MT 59812, United States*
[d]*Center for Biomolecular Structure & Dynamics, University of Montana, Missoula, MT 59812, United States*
[e]*Graduate School of Science, University of Hyogo, 3-2-1 Koto, Kamigori-cho, Ako-gun, Hyogo 678-1297, Japan*

Proteins fold into specific structures according to their amino acid sequences. However, there are many proteins that undergo three-dimensional domain swapping (3D-DS), a phenomenon in which a monomeric protein forms a dimer by exchanging the same domain or secondary structural element between molecules of the same protein [1]. We have shown that various heme proteins undergo 3D-DS [2]. We have also found that 3D-DS of heme proteins occurs at the early stage of protein folding, and utilized 3D-DS to construct various heme protein assemblies, including nanorings, cages, hetero dimers with different active sites, and a ligand-binding reversible monomer-polymer system [2].

Cytochrome *c* (cyt *c*) forms 3D-DS oligomers that exchanges the C-terminal α-helix between protomers [3]. This 3D-DS dimer was obtained by refolding the protein from a guanidium-ion unfolded state, where the N- and C-terminal regions interacted intermolecularly during folding [4]. In this study, we show that cyt *c* refolded from acidic and ethanol denatured states can fold into a same 3D-DS precursor state. The 3D-DS precursor state of cyt *c* showed a dimer-trimer equilibrium at high protein concentration (2 mM, heme unit) according to size exclusion chromatography. By X-ray crystallographic analysis of the 3D-DS precursor state of cyt *c*, we obtained a new 3D-DS dimer structure that exchanges the region beyond Asn54 between protomers. The dissociation rate of the cyt *c* 3D-DS precursor to monomers increased by the addition of apo cyt *c*, but not by the addition of holo cyt *c*, indicating that the 3D-DS precursor state is flexible. On the other hand, the cyt *c* dimer obtained by refolding without heat purification exhibited higher peroxidase activity than heat-purified dimer, indicating formation of an unstable dimer during folding which exhibits higher peroxidase activity than the 3D-DS precusor state. These results reveal the involvement of 3D-DS in folding of cyt *c*, showing that the flexible 3D-DS precursor state can fold into various 3D-DS structures.

REFERENCES

1. M. J. Bennett, M. P. Schlunegger, D. Eisenberg, *Protein Sci.*, **4**, 2455-2468 (1995).
2. S. Hirota, T. Mashima, N. Kobayashi, *Chem. Commun.*, **57**, 12074-12086 (2021).
3. S. Hirota, Y. Hattori, S. Nagao, M. Taketa, H. Komori, H. Kamikubo, Z. Wang, I. Takahashi, S. Negi, Y. Sugiura, M. Kataoka, Y. Higuchi, *Proc. Natl. Acad. Sci. USA*, **107**, 12854-12859 (2010).
4. P. P. Parui, M. S. Deshpande, S. Nagao, H. Kamikubo, H. Komori, Y. Higuchi, M. Kataoka, S. Hirota, *Biochemistry*, **52**, 8732-8744 (2013).

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Azahelicenes and triazahelicenes as Emerging Platforms for Low Band Gap Materials

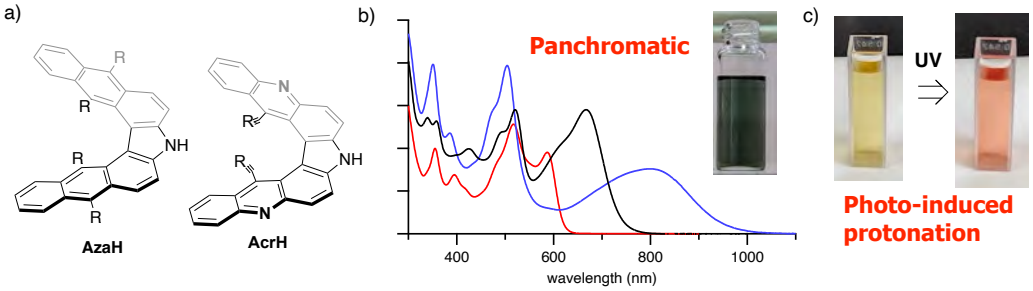
Satoru Hiroto, Moeko Chujo, Mana Wakita, Masahiko Fukumoto

Graduate School of Human and Environmental Studies, Kyoto University, Nihonmatsu-cho, Yoshida, Sakyo-ku, Kyoto 606-8501, Japan

Here, we will introduce our **useful curved-π units**, azahelicenes and triazahelicenes, which should contribute to the chemistry of porphyrins and phthalocyanines.

π-Conjugated molecules with low band gaps have attracted significant attention in materials science and photochemistry due to their near-infrared (NIR) absorption and emission properties. While numerous planar systems have been developed, examples of low-band-gap materials featuring ***curved*** π-surfaces remain challenging. Such architectures offer unique opportunities for chiroptical functionality, charge transport, and dynamic optical responses.[1)]

Our group has established efficient synthetic routes to π-extended aza[5]helicenes (**AzaH**), enabling gram-scale preparation and regioselective functionalization.[2)] Recently, we have achieved the first helicene-based polar crystals[3)] and revealed pitch-dependent optical properties in oxidized states. In addition, we developed donor–acceptor–donor (DAD) azahelicene dyads, which exhibit pronounced intramolecular charge-transfer interactions and panchromatic absorption extending into the NIR region.[4)] This study disclosed that the distortion of the π-plane caused biased molecular orbitals onto the helicene skeleton, inducing intramolecular charge transfer interaction even in the absence of an electron-accepting unit. This feature led to independent transitions between localized and charge-transfer transitions, serving panchromatic absorbing characteristics. Furthermore, we have synthesized triazahelicenes containing acridine skeletons (**AcrH**) as promising candidates for low-band-gap heterohelicenes. AcrH was synthesized via oxidative cyclization of 2-aminoacridine derivatives using Magic Blue. AcrH displayed luminescence and underwent protonation upon photoirradiation, enabling tunable photophysical behavior. In this presentation, we will discuss their synthesis, structure–property correlations, emphasizing their potential as curved π-systems for next-generation optoelectronic and photoresponsive materials.



REFERENCES

1. a) M. Saito, H. Shinokubo and H. Sakurai, *Mater. Chem. Front.* **2018**, *2*, 635. b) J. Labella, T. Torres, *et al. ChemistryEurope* **2025**, *Early View* (doi: 10.1002/ceur.202500244).
2. a) S. Hiroto, H. Shinokubo, *et al. Angew. Chem. Int. Ed.* **2012**, *51*, 10333. b) S. Hiroto, *Bull. Chem. Soc. Jpn.* **2018**, *91*, 829. c) S. Hiroto, *Bull. Chem. Soc. Jpn.* **2020**, *93*, 1334
3. S. Hiroto, M. Wakita, M. Chujo, *Chem. Asian. J,* **2022**, *17*, e202200808.
4. S. Hiroto, M. Chujo, *Chem. Asian. J.* **2025**, *20*, e202400830.

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Pyrrole-based anion-responsive macrocycles

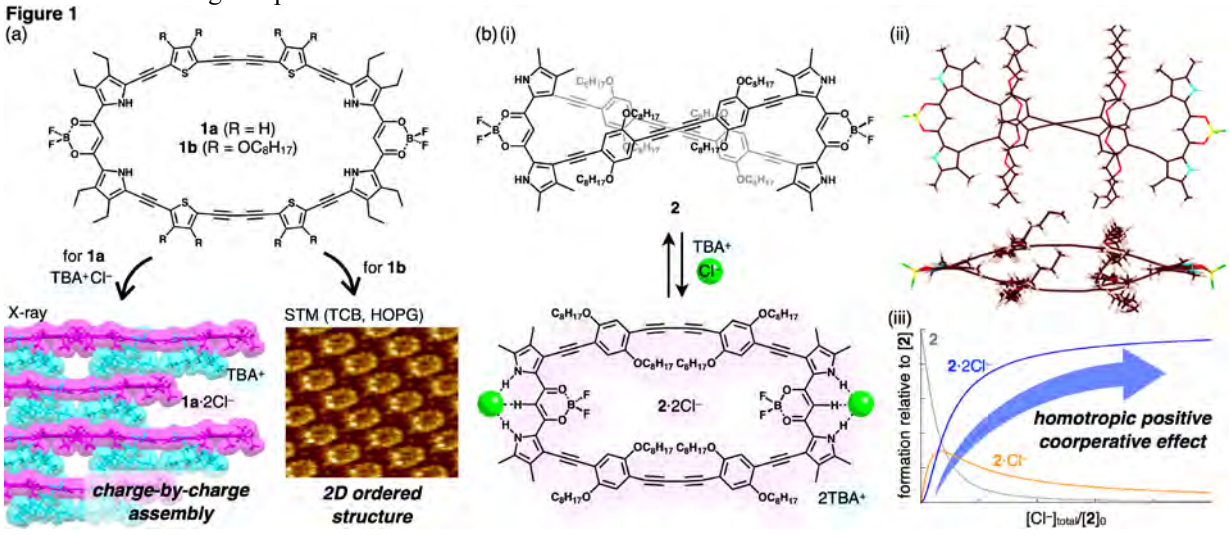
Hiroki Horita, Hiroki Okano, Yota Kawai, and Hiromitsu Maeda

Department of Applied Chemistry, College of Life Sciences, Ritsumeikan University, Kusatsu, 525–8577, Japan

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Dipyrrolyldiketone BF_2 complexes (PBs) are representative anion receptors that can form pseudo-π-electronic anions through the pyrrole-ring inversion accompanied by hydrogen bonding to anions at two pyrrolic NH sites and one bridging CH site. To date, anion-binding behavior and ion-pairing assembly of PBs and related molecules, as precursors of pseudo-π-electronic anions, have been reported [1]. Herein, we report characteristic properties of PB-based macrocycles. Macrocycles **1a**/**1b** (Figure 1a top) exhibited higher Cl^--binding affinity than the linear precursors, attributed to preorganized pyrrole-inverted states that are favorable for anion binding [1c]. Single-crystal X-ray analysis of **1a** upon the addition of TBACl revealed the complexation with two Cl^- at the anion-binding sites to provide the pseudo-π-electronic anion **1a**·2Cl^-, which formed a charge-by-charge assembly with two TBA^+ (Figure 1a bottom left). For macrocycle **1b**, scanning tunneling microscopy (STM) measurements on highly oriented pyrolytic graphite (HOPG) revealed a 2D ordered structure (Figure 1a bottom right). On the other hand, macrocycle **2**, with non-inverted pyrrole rings and crossed π-electronic linkers, was synthesized, showing the figure-eight shape structure in the X-ray structure (Figure 1b(i) top and (ii)). UV/vis absorption spectral changes in CH_2Cl_2 revealed the homotropic positive cooperative effect in Cl^- binding, arising from coupled pyrrole inversions of two PB units (Figure 1b(i) bottom and (iii)). Furthermore, stopped-flow measurements in CH_2Cl_2 (10 μM of **2** with 0.2 M of TBACl) revealed a remarkably slow anion-binding process, with the association reaching completion in ~10 s.

Figure 1



REFERENCES

1. (a) Haketa, Y.; Komatsu, K.; Sei, H.; Imoba, H.; Ota, W.; Sato, T.; Murakami, Y.; Tanaka, H.; Yasuda, N.; Tohnai, N.; Maeda, H. *Chem. Sci.* **2024**, *15*, 964. (b) Kugizaki, R.; Haketa, Y.; Kamada, K.; Maeda, H. *Chem. Eur. J.* **2024**, *30*, e202401932. (c) Horita, H.; Okano, H.; Kikkawa, Y.; Haketa, Y.; Maeda, H. *Chem. Asian J.* **2025**, *20*, e202401461. (d) Toyoshima, R.; Horita, H.; Tsuda, S.; Kobashi, S.; Kobayashi, H.; Kobayashi, Y.; Maeda, H. *Org. Lett.* **2025**, *27*, 7933.

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Development of low pH-activatable photosensitizers for photodynamic therapy and diagnosis

Hiroaki HORIUCHI[a,b]

[a]*Graduate School of Life and Environmental Sciences, Kyoto Prefectural University*
[b]*Graduate School of Science and Technology, Gunma University*

Photodynamic therapy (PDT) is a minimally invasive cancer treatment that induces tumor cell death through the generation of reactive oxygen species (ROS) upon photoexcitation of photosensitizers accumulated in tumor tissues. In addition to therapy, photodynamic diagnosis (PDD) can be achieved by exploiting the fluorescence of the photosensitizers used in PDT. Porphyrinoids have been clinically applied and represent promising chromophores for PDT and PDD. However, many conventional porphyrinoids inevitably accumulate in normal tissues, leading to undesired phototoxic side effects and reduced diagnostic accuracy due to background fluorescence. To overcome these limitations, activatable photosensitizers have attracted considerable attention. These photosensitizers remain in a photoinactive "OFF" state in normal tissues, thereby suppressing phototoxicity and background signals. In contrast, they switch to a photoactive "ON" state specifically within tumor tissues, enabling cancer-selective phototherapy and photodiagnosis [1]. Given that lysosomes exhibit an acidic microenvironment, the combination of low pH-activatable photosensitizers with lysosome-targeting drug delivery systems represents a promising strategy for highly cancer-selective PDT and PDD. In this study, we aim to develop efficient low pH-activatable photosensitizers for improved cancer-selective phototheranostic applications.

Aromatic amines have been introduced into the meso position of porphyrins as pH-responsive quenchers. A derivative with a diethylaniline exhibited a low fluorescence quantum yield Φ_f and quantum yield of singlet oxygen ($^1O_2$) production Φ_Δ under neutral conditions due to rapid deactivation from the charge-transfer excited state. In contrast, under acidic conditions, the quenching ability of the aniline unit was lost upon protonation, resulting in switching to the ON state with high Φ_f and Φ_Δ. However, this derivative slightly sensitize $^1O_2$ even in neutral solution and the ON/OFF ratio of Φ_Δ was low (11) [2].

To improve the ON/OFF ratio, we developed AI4P which is a porphyrin derivative bearing four diethylaminoindole (AI) units [3]. In neutral solution, the first excited singlet state of AI4P was strongly quenched by the AI units, resulting in extremely weak fluorescence. Moreover, $^1O_2$ generation was not detected, and Φ_Δ was estimated to be below 0.002. In contrast, under acidic conditions, Φ_Δ increased markedly to 0.42, corresponding to an ON/OFF ratio exceeding 200. Notably, in acidic solution, a new intense absorption band appeared at 740 nm, which lies in the near-infrared region favorable for biological tissue penetration. While AI4P showed no absorption at this wavelength under neutral conditions, strong absorption emerged upon acidification, yielding an ON/OFF ratio of the molar extinction coefficient exceeding 400.

Because the amount of generated $^1O_2$ is approximately proportional to the product of the molar extinction coefficient and the quantum yield, the overall ON/OFF ratio of $^1O_2$ production was estimated to exceed 80,000. These results demonstrate that AI4P is a highly promising low pH-activatable photosensitizer for PDT. Further development of related porphyrin derivatives will also be discussed.

REFERENCES

1. N. Kwon et al., Angew. Chem. Int. Ed. 2025, 64, e202423348
2. H. Horiuchi et al., J. Photochem. Photobiol. A 2018, 365, 60.
3. H. Horiuchi et al., J. Photochem. PhotoBiol. A, 2020, 403, 112846.

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Targeted Nanotechnology and Microendoscopy for Photoimmunotherapy of Peritoneal Metastasis

Huang-Chiao Huang[a]

[a]*Fischell Department of Bioengineering, University of Maryland, College Park, MD 20742, USA*
[b]*Marlene and Stewart Greenebaum Cancer Center, University of Maryland School of Medicine, Baltimore, MD 21201, USA*

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Objectives: Fluorescence-guided interventions enhance standard therapies by enabling detection and treatment of microscopic tumors before lethal recurrence. Advances in photoimmunotherapy (PIT) show promise for intraoperative treatment of peritoneal metastasis. However, clinical translation remains difficult due to heterogeneous treatment responses. This study explores how nanotechnology and fluorescence-guided strategies can further improve PIT for peritoneal metastasis, potentially sensitizing tumors to hyperthermic intraperitoneal chemotherapy (HIPEC) [1].

Methods: We developed Targeted Photoactivable Multi-Agent Liposomes (TPMAL), a formulation combining nanoliposomal irinotecan with antibody–photosensitizer conjugates for synergistic PIT and chemotherapy. PIT is a two-step process: TPMAL administration followed by red light activation to generate reactive oxygen species (ROS) that kill cancer cells. Using the OVCAR-5 peritoneal metastasis mouse model, we evaluated TPMAL-PIT safety and efficacy. To optimize treatment, we developed two fluorescence-guided strategies:
(i) Fluorescence-Guided Drug Delivery (FGDD): Due to variable pharmacokinetics, optimal PIT timing varies across subjects. FGDD identifies peak TPMAL fluorescence in tumors to guide light activation.
(ii) Fluorescence-Guided Light Dosimetry (FGLD): Given intersubject TPMAL variability, FGLD monitors photosensitizer photobleaching during PIT, enabling real-time light dose adjustments for more consistent treatment.

Results: In mouse models of peritoneal carcinomatosis, TPMAL enhanced drug delivery to tumor nodules by 14-fold. The ML7710 clinical laser endoscopy system detected variability in TPMAL uptake and enabled real-time FGLD in over 50% of treated mice. TPMAL also improved photosensitizer penetration up to 3 mm in tumor nodules. Combining TPMAL, fluorescence-guided PIT, and irinotecan significantly reduced treatment variability and improved survival without systemic toxicity.

Conclusions:
This study integrates two innovations:
(i) TPMAL – a targeted, fluorescence-labeled nanoliposome platform for PIT and chemotherapy.
(ii) Fluorescence-guided interventions – for real-time visualization and patient-specific treatment.
Together, these technologies enable personalized light dosing and consistent PIT-chemotherapy outcomes—critical for treating heterogeneous peritoneal metastasis.

REFERENCES

1. Liang, B.J., et al., Fluorescence-guided photoimmunotherapy using targeted nanotechnology and ML7710 to manage peritoneal carcinomatosis. *Science Advances,* 2023. 9(36): p. eadi3441.

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Probing Charge Transport and Separation Mechanism in Porous Crystalline Frameworks

Jier Huang, Liangji Chen, James Wilkes

Department of Chemistry and Schiller Institute for Integrated Science and Society, Boston College, Chestnut Hill, MA 02617

Porous crystalline materials such as metal organic frameworks (MOFs) and covalent organic frameworks (COFs) represent a novel class of materials for catalysis due to their inherent porous nature, exceptional thermal and chemical stability, structural flexibility. While many optoelectronic and photocatalytic systems based on these materials have been developed in the past decade, a significant gap exists in our understanding of the correlation of photophysical and photochemical properties of MOFs/COFs with their structure, which hinders accurate prediction and informed design. We aim to address this challenge using an interdisciplinary approach that combines innovative material design and synthesis, and fundamental mechanistic studies by spectroscopic techniques. In this talk, I will discuss our recent progress in two projects including 1) understanding the charge transport mechanisms in 2D conductive MOFs and 2) developiong COFs as light harvesting and charge separation materials for photocatalytic applications.

2D conductive MOFs, an emerging class of porous solids, have recently attracted great attention due to their potential applications in energy storage devices, chemiresistive sensing, and quantum information. However, the fundamental understanding of the factors that control their conductive mechanism remains underexplored. In this talk, I will discuss a new strategy we used to controllably engineer their photoconductivity and charge transport (CT) pathway by systematically tuning the ligand size and metal nodes. Through a combination of hybrid synthesis with spectroscopic studies, we show that extending the ligand from single-benzene core to thirteen-benzene core can effectively control both intralayer π-d orbital overlap and interlayer π-π stacking interaction. This not only significantly affects their photo-conductivity but also shifts CT pathway from a through-bond dominated mechanism in smaller ligands to a through-space dominated mechanism in larger ligands, providing a versatile design strategy for directional CT. In addition, the photoconductivity is strongly influenced by the metal nodes, which can effectively alter the band gap and the dispersivity and ultimately photoconductivity.

Charge transfer process is one of the key factors that determine the efficiency of solar-driven CO_2 reduction into renewable fuels and valuable chemicals. Most photocatalytic CO_2 reduction systems reported require the use of sacrificial electron donor to participate in the catalytic process due to undesirable charge transfer pathways and low charge separation efficiency. Working towards economical CO_2 photoreduction necessitates replacement of sacrificial donors with ones that are abundant and easily accessible like H_2O. To address these issues, we have been developing chemical approaches to control charge transfer pathways in COFs, where the wide availability of diverse functional building blocks allows the precise tuning of its structure and functional components. We hope to use this strategy as a crucial tool to make H_2O a potentially suitable electron donor which could eventually make solar-driven CO_2 photoreduction economically feasible.

REFERENCES

1) J. Am. Chem. Soc. 2020, 120, 21050-21058
2) J. Am. Chem. Soc. 2024, 146, 4489-4499

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Metal Complexes of N-Confused Porphyrins and Their Sustainable Energy Applications

Chen-Hsiung Hung[a], Tanmoy Pain[a], Kai-Chun Hsi[b], Bhakyaraj Kasi[a], Belarani Ojha[a]

[a]*Institute of Chemistry, Academia Sinica, Nankang, Taipei 115201, Taiwan*
[b]*Department of Chemistry, National Taiwan University, Taipei 106319, Taiwan*

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The development of N-confused porphyrins and their derivatized analogues, together with their metal complexes, has significantly enriched the chemistry of porphyrinoids. Beyond fundamental coordination chemistry, this class of macrocycles has found expanding applications in molecular sensing, imaging, medicinal chemistry, and catalysis.[1-2] In response to urgent global demands for sustainable energy conversion and carbon-neutral technologies, this lecture will highlight the emerging potential of N-confused porphyrin metal complexes in electrocatalytic carbon dioxide reduction (eCO_2RR) and nitrate reduction (eNO_3RR).

The presentation will begin with our recent studies on vanadium N-confused porphyrins,[3] focusing on their unique electronic structures and catalytic oxygenation reactivity. We will then discuss the electrocatalytic conversion of CO_2 to formate mediated by tin(IV) N-confused porphyrin complexes, followed by iron N-confused porphyrin systems as catalysts for nitrate-to-ammonia conversion operated in gas-diffusion-based flow electrochemical cells. Collectively, these studies demonstrate that N-confused porphyrin complexes can deliver effective and selective electrocatalytic activity for both eCO_2RR and eNO_3RR. The chemistry presented underscores the promise of N-confused porphyrins as structurally programmable molecular platforms for sustainable electrocatalytic transformations that convert greenhouse gases and environmental pollutants into value-added chemical feedstocks.

REFERENCES

1. Toganoh, M.; Furuta, H. *Chem. Rev.* **2022**, *122*, 8313–8437.
2. Bialek, M. J. ; Hurej, K. ; Furuta, H. ; Latos-Grazynski, L. *Chem. Soc. Rev.* **2023**, *52*, 2082-2144.
3. Kasi, B.; Peng, S.-H.; Ambre, R.; Lin, S.-C.; Chen, T.-T.; Pain, T.; Hsu, K.-C.; Liaw, W.-F.; Ojha, B.; Hung, C.-H. *J. Porphyr. Phthalocyanines*, **2025**, *29*, 229-241.

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The unusual chemistry of pyriporphyrins - from controlled ring inversion to pyridine ring contraction

Karolina Hurej, Paulina Krzyszowska, Michał J. Białek, Lechosław Latos-Grażyński[a]

[a]*University of Wroclaw, Department of Chemistry, F. Joliot-Curie 14, 50383 Wrocław (Poland), e-mail: karolina.hurej@uwr.edu.pl*

The coordination chemistry of carbaporphyrinoids has become a popular area of research in recent years. These macrocycles are of great interest due to the formation of complexes in which metals acquire unusual oxidation states and subsequently exhibit non-trivial reactivity associated with the formation of organometallic bonds. Despite numerous studies, the coordination chemistry of pyriporphyrins - macrocycles in which one of the pyrrole rings has been replaced by a pyridine ring - remains poorly understood. However, studies of the reactivity of pyriporphyrins, regardless of how the six-membered ring is incorporated, demonstrate the fascinating nature of this chemistry [1-3].

One such example is di-*p*-pyrirubyrin. During stepwise acid titration, we observed the inversion of one or two six-membered rings. Consequently, three fundamental conformers are feasible: regular, N-confused, and doubly N-confused, which provide principal sites preadapted for further protonation [4]. Additionally, di-*p*-pyrirubyrin complexes with palladium(II) ions exhibit a response in photoacoustic spectroscopy [5].

Another case is 3-aza-*meta*-benziporphyrin, in which the pyridine ring contracts to form the pyrrole ring. By investigating the unusual coordination chemistry of N-confused pyriporphyrin with silver and gold ions, we observed this process and obtained several complexes that exhibited remarkable reactivity. This includes the reversible cleavage of C–O bonds and the selective demetallation of the outer metal ion [6].



REFERENCES

1. M. Das and A. Srinivasan, *Chem. Commun.*, **2023**, *59*, 11780-11790.
2. T. D. Lash, *Chem. Rev.*, **2017,** *117*, 2313-2446.
3. K. Hurej and L. Latos-Grażyński, *A Pincer Motif Etched into a meta-Benziporphyrin Frame*, in *Metal-Ligand Co-operativity: Catalysis and the Pincer-Metal Platform*, G. van Koten, K. Kirchner, and M.-E. Moret, Editors. **2021**, Springer International Publishing: Cham. p. 181-225.
4. R. Myśliborski, K. Hurej, M. Pawlicki, L. Latos-Grażyński, *Angew. Chem. Int. Ed.* **2018**, *57*, 16866-16870
5. K. Hurej, W. Oszczęda, E. Opas, S. J. Zelewski, M. Pawlicki, M. J. Białek, Ł. Orzeł, L. Latos-Grażyński, *Angew. Chem. Int. Ed.* **2023**, *62*, e202303394
6. P. Krzyszowska, A. Burska-Jabłońska, M. Oberski, M. J. Białek, L. Latos-Grażyński, K. Hurej, *Angew. Chem. Int. Ed.* **2026**, e25506.

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Electroabsorption Spectroscopy of BOPHY Derivatives: Probing Charge Transfer Character in the Excited State

Md. Bulu Rahman[a], Victoria Villarreal[b], Victor N. Nemykin[b], Toshifumi Iimori[a]

[a]*Department of Sciences and Informatics, Muroran Institute of Technology, Muroran, Japan*
[b]*Department of Chemistry, University of Tennessee – Knoxville, Knoxville, TN USA*
iimori@muroran-it.ac.jp

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In organic light-harvesting systems, the most widely employed electron acceptors have been fullerene and its derivatives. Organic photovoltaics (OPVs) employing novel non-fullerene electron acceptors (NFAs) have shown improved performance in terms of stability and efficiency compared to OPVs using conventional fullerene derivatives. Recent studies of a high-performance NFA Y6 have shown that its efficient charge generation in the donor – acceptor system is linked to charge transfer (CT) excitations within the NFA. As potential NFAs for light-harvesting systems, BOPHY chromophores have also attracted a great deal of attention because of their tunable photophysical and redox properties. Here, electroabsorption (EA) spectroscopy of a series of BOPHY derivatives is reported. EA spectroscopy is a powerful spectroscopic technique to probe the CT character of chromophores through the quantification of the changes in electric dipole moment and polarizability volume between the excited and ground states [1-5]. The correlation of the CT character of the excited state with the substitution groups will be discussed.

REFERENCES

1. Rahman, M. B.; Islam, A.; Iimori, T. Exciton Delocalization and Polarizability in Perylenetetracarboxylic Diimide Probed Using Electroabsorption and Fluorescence Spectroscopies. *Molecules* **2024**, *29,* 2206.
2. Islam, A.; Syundo, K.; Iimori, T. Charge-Transfer State and State Mixing in Tetracyanoquinodimethane Probed Using Electroabsorption Spectroscopy. *Phys. Chem. Chem. Phys.* **2023**, *25*, 21317-21323.
3. Islam, A.; Kikuchi, Y.; Iimori, T. Electroabsorption and Stark Fluorescence Spectroscopies of Thioflavin T. *J. Phys. Chem. A* **2023**, *127*, 1436-1444.
4. Iimori, T.; Ito, R.; Ohta, N.; Nakano, H. Stark Spectroscopy of Rubrene. I. Electroabsorption Spectroscopy and Molecular Parameters. *J. Phys. Chem. A* **2016**, *120*, 4307-4313.
5. Iimori, T.; Ito, R.; Ohta, N. Stark Spectroscopy of Rubrene. II. Stark Fluorescence Spectroscopy and Fluorescence Quenching Induced by an External Electric Field. *J. Phys. Chem. A* **2016**, *120*, 5497-5503.

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Engineering Porphyrins and Redox Mediators for Enhanced Dye-Sensitized Solar Cell Performance

Hiroshi Imahori[a-c]

[a]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University*
[b]*Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University*
[b]*Institute of Liberal Arts and Sciences (ILAS), Kyoto University*

Porphyrin dyes continue to attract significant interest as high-performance photosensitizers for dye-sensitized solar cells (DSSCs), particularly when paired with cobalt(II/III) complex-based redox shuttles, achieving excellent light-harvesting and power conversion efficiencies (PCEs). Recently, copper(I/II) complexes have emerged as next-generation redox shuttles, offering impressive open-circuit voltages (V_{OC}) exceeding 1.0 V. However, porphyrin-based DSSCs incorporating copper(I/II) shuttles have faced challenges in achieving high PCEs, largely due to insufficient driving force for efficient dye regeneration. We present FL1—a newly designed porphyrin dye featuring a fluorene moiety with reduced electron-donating characteristics—to address this limitation. FL1 was engineered to enhance the driving force for dye regeneration by copper(I/II) complexes. Under optimized conditions, DSSCs utilizing FL1 and the copper(I/II) complex $[Cu(2MeOby)_2]^+/[Cu(2MeOby)_2]^{2+}$ with trifluoromethanesulfonimide ($TFSI^-$) counterions achieved a notable PCE of 8.30% and a V_{OC} of 0.890 V. Further investigation into counterion effects revealed that replacing $TFSI^-$ with hexafluorophosphate (PF_6^-) significantly improved performance, yielding a PCE of 9.06% and a V_{OC} of 0.900 V, attributed to enhanced diffusion properties. Moreover, co-sensitization with FL1 and a complementary dye XY1B led to a record-breaking PCE of 10.9%, while maintaining a high V_{OC} of 0.945 V—setting a new benchmark for porphyrin-based DSSCs with copper(I/II) redox shuttles. These findings underscore the transformative potential of energy-level engineering in porphyrin dyes and copper-based redox systems to optimize dye regeneration and drive future advancements in DSSC technology. In this presentation, I will provide an overview of our design strategies, experimental insights, and the implications of our findings for next-generation DSSC development.

REFERENCES

1. T. Higashino, H. Imahori, *ACS Energy Lett.* (Perspective), **7**, 1926-1938 (2022).
2. H. Imahori, *Bull. Chem. Soc. Jpn.* (Award account), **96**, 339-352 (2023).
3. Y. Zhang, T. Higashino, H. Imahori, *J. Mater. Chem. A* (Review), **11**, 12659-12680 (2023).
4. H. Imahori, M. Akiyama, *J. Porphyrins Phthalocyanines* (Award account), **28**, 321-337 (2024).
5. Y. Kurumisawa, T. Higashino, S. Nimura, Y. Tsuji, H. Iiyama, H. Imahori, *J. Am. Chem. Soc.*, **141**, 9910-9919 (2019).
6. Y. Zhang, T. Higashino, I. Nishimura, H. Imahori, *ACS Appl. Mater. Interfaces*, **16**, 67761-67770 (2024).
7. Y. Zhang, T. Higashino, K. Namikawa, W. R. Osteloh, H. Imahori, *Chem. Sci.*, **16**, 15004-15014 (2025).

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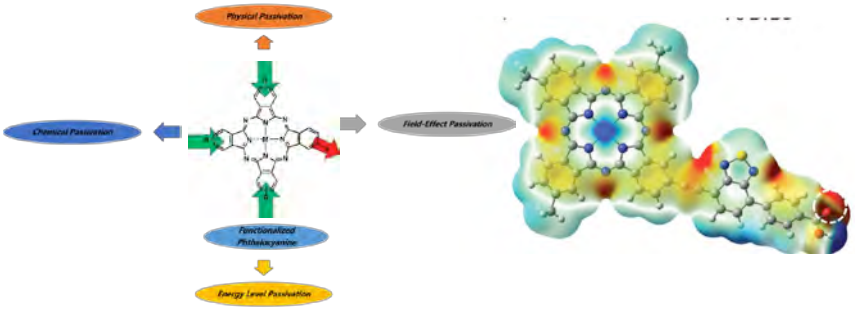
Multifunctional Phthalocyanine-Based Hole Transport and Interfacial Passivation Materials for Perovskite Solar Cells

Mine Ince[a], Perihan Kübra Demircioglu[a], Murat Ebic [b], Şifa Dogan[a] ,Seckin Akin [b]

[a] *Department of Natural and Mathematical Science, Tarsus University, Mersin, 33400, Turkey*
[b] *Laboratory of Advanced Materials &Photovoltaics (LAMPs), Necmettin Erbakan University, Konya 42090, Turkey;*

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Perovskite solar cells (PSCs) have rapidly emerged as one of the most promising photovoltaic technologies, achieving power conversion efficiencies (PCEs) exceeding 26% within just a decade. Although the recent skyrocketing advances in PSCs approach the conventional inorganic technologies, the ionic nature, as well as extrinsic factors, endow perovskite crystals with a large number of defects, including undercoordinated ions at crystal surfaces and at the grain boundaries, which act as non-radiative recombination centers both within photoactive layers and at electrode contacts, resulting in low Voc, PCE, and degradation of the device. [1]To circumvent the severe issue, passivating and/or healing these defects on the perovskite surface and grain boundaries (reducing the non-radiative recombination loss) are among the most promising approaches to improving the stability and efficiency of both perovskite solar cells. Pcs, planar aromatic macrocycles and p-type semiconductors, are well known as efficient hole-transporting materials (HTMs). [2] While most studies on Pcs in PSCs have focused on their role as HTM alternatives to spiro-OMeTAD—achieving impressive efficiency and stability—their exceptional photophysical properties, charge-transport capabilities, and highly tunable chemical structures have increasingly encouraged their use as functional additives to control perovskite film crystallization, reduce defect densities, and enhance charge transport and extraction.[3] In this talk, we will present our recent findings on Pc–based multifunctional passivators and HTMs for PSCs. We will highlight their dual role as efficient HTMs and defect-passivating agents, and discuss how functionalized Pc derivatives can be tailored to address different requirements for achieving high-efficiency and long-term stable PSCs.



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REFERENCES

1. Wang, J.; Bi, L.; Fu, Q.; Jen, A. K. Y. Adv. Energy Mater. 2024, 14 (35), No. 2401414.
2. Urbani, M.; de la Torre, G.; Nazeeruddin, M. K.; Torres, T. Chem. Soc. Rev. 2019, 48 (10), 2738−2766
3. C. Li, S. Dogan, Y. Li, H. Zhang, S. Tang, Z. Yuan, L. Liang, Z. Zhang, Y. Wang, C. Liu, Y. Yang, M. Ince, and P. Gao, P. Advanced Energy Materials, 15 (2025): 2402856.

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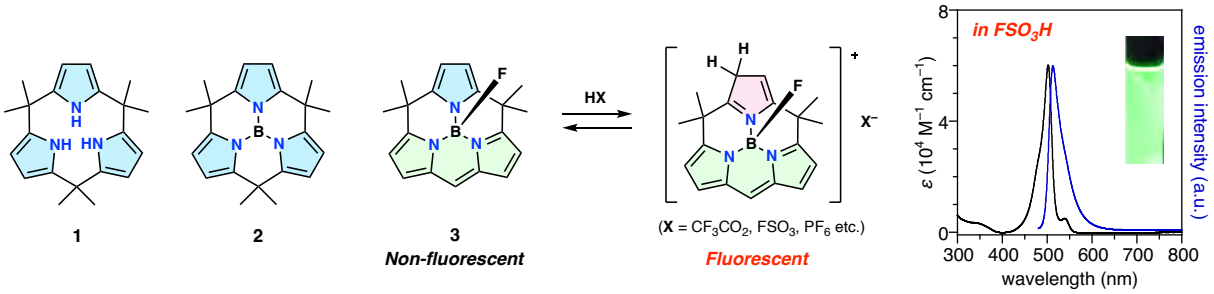
Superacid-Resistant Macrocyclic BODIPYs Inspired by Boron–Calix[3]pyrrole

Yasuhide Inokuma[a,b]

[a]*Division of Applied Chemistry, Faculty of Engineering, Hokkaido University, Japan*
[b]*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University*

Boron–dipyrromethene (BODIPY) dyes are well-known fluorophores that show bright visible emission with narrow Stokes shifts. Despite their diverse applications in staining and sensing, BODIPYs have suffered from a common drawback; they readily release the boron atom under acidic conditions, leading to fluorescence degradation. In the course of our research on calix[3]pyrrole,[1] we discovered unusual protonation behavior and a synergistic effect in boron chelation by the tripyrrolic macrocycle, which provided a rational molecular design for superacid-stable BODIPY dyes.

While calix[3]pyrrole (**1**) undergoes an acid-catalyzed, strain-induced ring expansion reaction via irreversible macrocyclic ring cleavage, its boron complex **2** is reversibly protonated at the pyrrole *β*-position without undergoing deboronation. When the BODIPY framework was embedded into a calix[3]pyrrole-like macrocycle bearing one sp^2-hybridized *meso*-carbon bridge, similar protonation behavior was observed for the macrocyclic BODIPY **3**. BODIPY **3** was synthesized in 46% yield by the condensation of boron-tripyrrane complex in triethyl orthoformate.[2] Upon protonation with trifluoroacetic acid (TFA), the π-conjugationally isolated pyrrole unit in **3** underwent protonation at the *β*-position to lead 3*H*-pyrrole ring, while the BODIPY unit remained unchanged. Although the fluorescence of **3** was quenched under neutral conditions due to photo-induced intramolecular electron transfer from the pyrrole moiety to the BODIPY core, its protonated state exhibited yellowish fluorescence at 549 nm with a quantium yield of 0.81 and a Stokes shift of 371 cm^{-1} in non-diluted TFA. Interestingly, no deboronation was observed even in absolute superacids such as chlorosulfonic acid and trifluoromethanesulfonic acid, and intense fluorescence was preserved with quantum yields of up to 0.90 (in fluorosulfonic acid). The superacid-resistant BODIPY **3** was utilized for staining strongly acidic materials, including Nafion and sulfonylated organo gels, as a fluorescent acid indicator. BODIPY **3** complements existing BODIPY analogues by enabling staining and sensing in strongly acidic environments, thereby expanding the functional scope of the BODIPY dye family.



REFERENCES

1. Y. Inaba, Y. Nomata, Y. Ide, J. Pirillo, Y. Hijikata, T. Yoneda, A. Osuka, J. L. Sessler, Y. Inokuma, *J. Am. Chem. Soc.* **2021**, *143*, 12355.
2. K. Watanabe *et al*. *Manuscript in revision*.

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N-bridged dimeric porphyrinoids

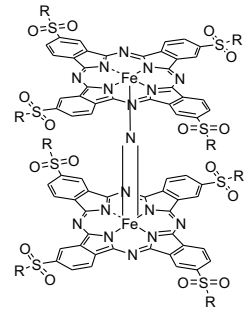
Ümit İşci[a]

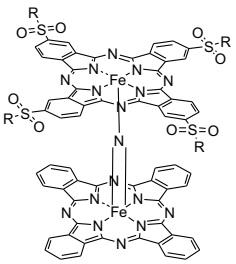
[a] *Marmara University, Faculty of Technology, Department of Metallurgical & Materials Engineering, 34722 Istanbul, Türkiye*

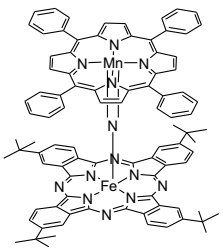
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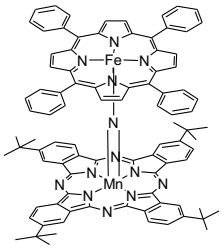
N-bridged dimeric porphyrinoids are very peculiar derivatives, in which two porphyrinoid macrocycles metalated with iron, ruthenium, manganese, chrome or rhenium are bridged by a single nitrogen atom [1-3]. They are known to be powerful oxidation catalysts, especially when compared to their monomeric components. N-bridged dimeric porphyrinoids have shown significant catalytic properties for oxidation of methane [4], benzene [5], alkyl aromatics [6], and alcohols [7].

N-bridged dimeric phthalocyanine complexes as oxidation catalysts will be discussed.









REFERENCES

1. A. B. Sorokin, *Chem. Rev.* **2013**, *113*, 8152.
2. Ü.İşci, F. Dumoulin, A. Sorokin and V. ahsen, *Turk. J. Chem*. **2014**, *38*, 923.
3. Z. Şahin, Ç. Yüceel, D. B. Yildiz, Y. Dede, F. Dumoulin and Ü. İşci, *Mol. Catal*. **2024**, *559*, 113986.
4. A. B. Sorokin, E.V. Kudrik and D. Bouchu, *Chem. Commum*. **2008**, 2562.
5. A. B. Sorokin, E.V. Kudrik, *Chem. Eur. J*. **2008**, *14*, 7123.
6. Ü. İşci, P. Afanasiev, Jean-Marc M. Millet, E. V. Kudrik, V. Ahsen and A. B. Sorokin, *Dalton Trans.* **2009**, 7410.
7. Ç. Yüceel, Z. Şahin, D. B. Yildiz, Y. Dede, F. Dumoulin and Ü. İşci, *J. Catal.* **2025**, *450*, 116220.

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N-Confused Bilatriene as a Versatile Scaffold for Metal–π Conjugated Porphyrinoids

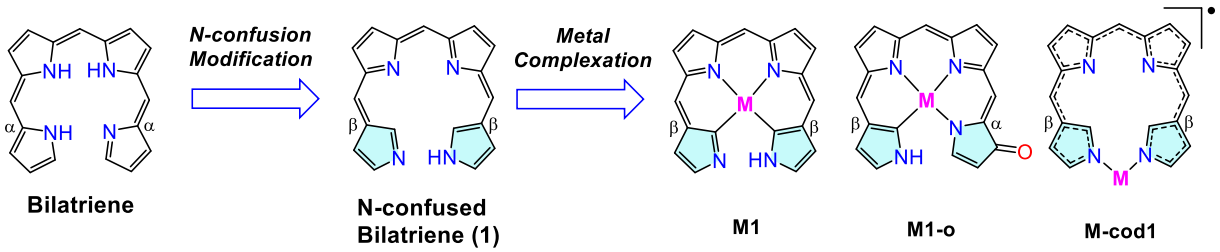
Masatoshi Ishida

Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University, Hachioji 192-0397 Japan
Email: ishidam@tmu.ac.jp

Open-chain tetrapyrrolic compounds derived from the porphyrin skeleton, including bilirubin, are known as bile pigments and represent potential ligand platforms for advanced dye applications. Owing to their flexible, linear π-conjugated frameworks, these molecules can undergo dynamic conformational and electronic modulation through metal-ion coordination. This feature endows them with remarkable tunability in their optical responses, making them promising photoactive materials that exhibit distinctive absorption properties extending into the second near-infrared (NIR-II; 1000–1700 nm) region.[1]

Recently, we have synthesized metal-bridged bilatriene complexes (**M1** and **M1-o**) coordinated with palladium(II) and platinum(II) ions,[2,3] and demonstrated that N-confusion structural modification of the ligand significantly enhances the interaction between the ligand π orbitals and the metal d orbitals. As a result, this approach enables the design of highly stable near-infrared dyes possessing exceptionally narrow HOMO–LUMO gaps. Furthermore, complexation of iridium(I) and rhodium(I) fragments at the outer indole-nitrogen sites of an N-confused bilatriene produces neutral π-radicaloid species (**M–cod1**) with delocalized spins and open-shell doublet ground states.[4] These complexes display broad NIR-II absorption bands extending up to 1500 nm and exhibit strong photoacoustic and photothermal responses arising from SOMO–SUMO-based transitions.

Together, these studies demonstrate that N-confused bilatriene serves as a versatile molecular scaffold for constructing both closed-shell metalla-carbaporphyrinoids and open-shell metal-bridged radicaloid systems.



REFERENCES

[1] H. Furuta, M. Ishida *et al., ChemPlusChem*, **2025**, *90*, e202500090.
[2] J. Kim, M. Ishida, and H. Furuta *et al., Angew. Chem. Int. Ed.* **2024**, *63*, e202405059.
[3] B. Basumatary, H. Furuta, M. Ishida, *et al., J. Porphyrins Phthalocyanines*, **2025**, *29*, 93-100.
[3] T. Ikeue, H. Furuta, M. Ishida *et al. Angew. Chem. Int. Ed*. **2025**, *64*, e202418751.

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Cryo-EM structure of monomeric bovine cytochrome *c* oxidase in a lipid nanodisc

Izumi Ishigami[a], Gabriella Angiulli[b], Joshua H. Mendez[b], Syun-Ru Yeh[a] and Denis L. Rousseau[a]

[a]*Department of Biochemistry, Albert Einstein College of Medicine, 1300 Morris Park Ave, Bronx, NY 10461 USA*
[b]*National Resource for Automated Molecular Microscopy, Simons Electron Microscopy Center, 89 Convent Ave, New York, NY 10027 USA*

Cytochrome *c* oxidase (C*c*O) is an essential enzyme in mitochondrial and bacterial respiration. It catalyzes the four-electron reduction of molecular oxygen to water and harnesses the chemical energy to translocate four protons across biological membranes, thereby establishing the proton gradient required for ATP synthesis. X-ray crystallographic structure analyses of bovine C*c*O (bC*c*O) have been based mainly on the dimeric form of the enzyme[1,2]. Recent cryogenic-electron microscopy (cryo-EM) structures revealed that C*c*O exists in its monomeric form in the respiratory supercomplex[3,4,5]. By treating the enzyme with TritonX-100, we generated the monomeric form of bC*c*O in solution and embedded it into nanodiscs for cryo-EM imaging. The nanodisc is comprised of a membrane scaffold protein (MSP), which encircles a lipid center providing a native-like environment for bC*c*O. We obtained a single particle cryo-EM structure of bC*c*O and resolved it to a overall resolution of 1.96 Å (local resolution of 1.90 Å). Here we will compare this single particle monomeric cryo-EM structure to those of the monomeric and dimeric structures of bC*c*O obtained by X-ray crystallography and compare the activity of monomeric bC*c*O embedded in a nanodisck to those obtained in solution.

REFERENCES

1. Izumi Ishigami et al. Proc Nat Acad Sci (USA) 2019, 116, 3572-3577.
2. Soo Jae Lee et al. Acta Cryst. 2001, D57, 941-947
3. Jinko Gu et al. Nature. 2016, 537, 639-643.
4. James A Letts. et al. Nature. 2016, 537, 644-648.
5. Wan Zheng et al. Nature. 2024, 631(8019), 232-239

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Direct Observation of the $S_0 \rightarrow T_n$ Transitions in Porphyrin Complexes, Evidenced by Magnetic Circular Dichroism

Kazuyuki Ishii[a]

[a] *Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba Meguro-ku, Tokyo, 153-8505 Japan.*

ORALS

Studies involving molecular excited triplet states have attracted considerable attention in terms of controlling the spin multiplicity, which is believed to help overcome some limitations for light utilization from the viewpoint of triplet precursor-based organic light emitting diodes, triplet-triplet annihilation-based energy upconversion, singlet fission, singlet-triplet absorption-based photochemical reactions, or solar cells, photocatalysts, phosphorescent O_2 sensors, and singlet oxygen generators. Therefore, over the past decade, it has become increasingly important to understand excited triplet states due to their potential applications in the design and development of photofunctional molecules. In this study, we investigated the excited triplet states of porphyrin complexes using electronic absorption, magnetic circular dichroism (MCD), and emission spectroscopies.

1) In an iridium(III) phthalocyanine (IrPc) complex, the introduction of the iridium(III) centre, which possesses strong spin-orbit coupling, induced the appearance of transitions between the singlet ground (S_0) state and the lowest excited triplet (T_1) state ($S_0 \leftrightarrow T_1$). In addition to two Faraday *A* terms corresponding to the Q- and B-bands, a third Faraday *A* term was successfully observed for the $S_0 \rightarrow T_1$ transition, indicating that the T_{1x} and T_{1y} states were degenerate in accordance with the expected D_{4h} symmetry of the π-conjugated system of IrPc [1].

2) Since the second lowest excited triplet (T_2) state is known to play an important role in enhancing the non-radiative intersystem crossing (ISC) process from the lowest excited singlet (S_1) state to the T_1 state, it is strongly desired to develop direct observation methods for the non-luminescent, short-lived T_2 state. At low temperature, in a highly concentrated solution of a platinum(II) octaethylporphyrin (PtOEP) complex, we successfully observed a distinct Faraday *A* term for the $S_0 \rightarrow T_1$ transition, as well as for the $S_0 \rightarrow T_2$ transition [2].

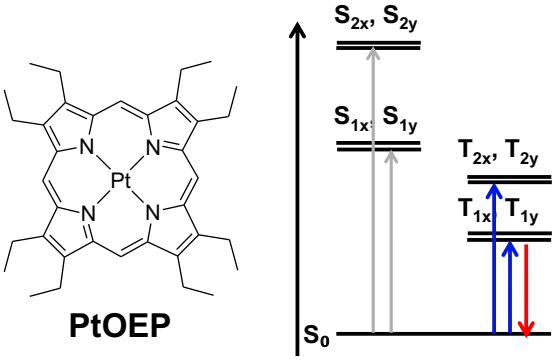


Figure 1. Molecular structure of PtOEP and its excited states.

The novel spectroscopic methodology applied allows resolution of the excited-state properties of a wide variety of transition-metal complexes.

REFERENCES

1. K. Murata, K. Ishii, *Eur. J. Inorg. Chem.*, **44**, 5103-5107 (2017).
2. K. Ishii, J. Wada, K. Murata, *J. Phys. Chem. Lett.*, **11**, 9828-9833 (2020).

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Exploring the 4f–π Coupling in Lanthanide Porphyrinoids: Insights from Magneto-Optical Spectroscopy

Naoto Ishikawa[a]

[a]*Department of Chemistry, The University of Osaka*

ORALS

The study of lanthanide porphyrinoids has been a journey of constant surprises. Since our early work in 2003 on the 4f electronic structures [1] and single-molecule magnet (SMM) behavior of double-decker complexes [2,3], these systems have served as a fascinating platform for exploring molecular magnetism. While these initial findings ignited a vastly extended search within the molecular magnetism community for new lanthanide-based SMMs and their potential applications in molecular spintronics and quantum computing, our research focus shifted. We became interested in how the lanthanide center communicates with its organic environment—an investigation that we have since extended from ground-state single-molecule magnetism of 4f elements to the photo-induced magnetism of 4f-π multi-angular-momentum systems.

With the hope that the localized 4f electronic system would communicate with the circular π-conjugated system of porphyrinoids via photo-excitation, we began investigating the Variable-Temperature Variable-Field Magnetic Circular Dichroism (VT-VH-MCD) of these 4f-π systems. Indeed, the bis(phthalocyaninato)terbium and dysprosium SMMs were found to exhibit surprisingly intriguing behaviors that do not appear at room temperature: specifically, large temperature dependence and non-linear magnetic-field dependence of the MCD profiles of the π-π* bands. They exhibit either an increase or decrease (followed by a reversal) of MCD A-term intensity upon cooling to cryogenic temperatures, as well as non-linear magnetic-field dependence, including the reversal of the MCD profile depending on the combination of the metal and the π-π* excited state [4,5].

A theoretical model where the total angular momentum of the 4f system (J) and the orbital angular momentum of the photo-excited π system of the macrocyclic ligand (L) are coupled—which we denote as J–L coupling—well describes the MCD behavior. This model provides clear insight into the ferromagnetic- or antiferromagnetic-type alignment of the two angular momenta.

In this talk, I will share our progress in the research of these multi-angular-momentum systems, including single-, double-, and triple-decker porphyrinoid-lanthanide complexes. While our theoretical model is still evolving and does not yet explain every experimental detail, it has been a helpful guide in interpreting the phenomena we observe across a range of phthalocyanine and porphyrin systems. I will conclude by reflecting on the long-term possibilities of these materials. While the deterministic manipulation of 4f quantum states via light remains a distant goal—a "dream" for the future—the steps we are taking today to understand the fundamental J–L mechanism are, I hope, a meaningful part of that larger pursuit toward molecular quantum technologies.

REFERENCES

1. N. Ishikawa, M. Sugita, T. Okubo, N. Tanaka, T. Iino, Y. Kaizu, *Inorg. Chem.* 2003, 42, 7, 2440-2446.
2. N. Ishikawa, M. Sugita, T. Ishikawa, S. Koshihara, Y. Kaizu, *J. Am. Chem. Soc.* 2003, 125, 29, 8694-8695.
3. N. Ishikawa, M. Sugita, W. Wernsdorfer, *Angew. Chem. Int. Ed.* 2005, 44, 19, 2931-2935.
4. K. Kizaki, H. Ozawa, T. Kobayashi, R. Matsuoka, Y. Sakaguchi, A. Fuyuhiro, T. Fukuda, N. Ishikawa, *Chem. Commun.* 2017, 53, 6168.
5. T. Fukuda, H. Ozawa, Y. Sakaguchi, K. Kizaki, T. Kobayashi, A. Fuyuhiro, N. Ishikawa, *Chem. Eur. J.* 2017, 23, 16357.

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Conformational Gating Mechanism in Electron Transfer Reaction from Cytochrome *c* to Cytochrome *c* Oxidase

Koichiro Ishimori

Department of Chemistry, Faculty of Science, Hokkaido University

ORALS

Electron transfer (ET) between cytochrome *c* (Cyt *c*) and cytochrome *c* oxidase (C*c*O) is a key step in cellular respiration, coupling electron flow to proton pumping across the mitochondrial membrane. Despite extensive structural and kinetic studies, the precise mechanism governing ET between these proteins remains unresolved, particularly regarding the role of protein dynamics and complex formation. In this study, we combined temperature-dependent flow-flash spectroscopy with computational modeling to elucidate the molecular basis of ET from Cyt *c* to C*c*O, revealing a conformational gating mechanism that regulates ET efficiency [1]. We measured the intracomplex ET rate constant (k_{ET}) between Cyt *c* and C*c*O using flow-flash spectroscopy, and the rapid phase of Cyt *c* oxidation exhibited a rate of approximately 10^4 s^{-1}, corresponding to an ET distance of 12.9–13.9 Å as estimated by Marcus theory. This distance is significantly shorter than the ~23 Å separation observed in the canonical enzyme-substrate (ES) complex by docking simulations [2]. The discrepancy indicates that ET does not occur in the most energetically stable ES complex but rather in a distinct ET-active complex characterized by a shorter donor–acceptor distance. Importantly, k_{ET} is ~80 times faster than the catalytic constant ($k_{cat} \approx 10^2$ s^{-1}), demonstrating that ET is not the rate-limiting step. Instead, the overall reaction is controlled by a conformational transition from the ES complex to the ET-active complex, occurring on the millisecond timescale. To identify the structural basis of the ET-active complex, we performed protein-protein docking and molecular dynamics (MD) simulations under constraints derived from experimental ET distances. Among candidate models, a model exhibited the shortest Fe–Cu_A distance (~17.9 Å) and the most favorable ET pathway. Pathways analysis revealed that this model provides the largest electronic coupling and shortest tunneling route, supporting its role as the ET-active configuration. Hydrophobic residues surrounding the exposed heme periphery of Cyt *c*, notably Ile81 and Val83, form a "molecular breakwater" that stabilizes ET-active complexes by excluding water molecules from the ET interface. Site-directed mutagenesis replacing Ile81 with serine (I81S) increased the ET distance by ~4 Å and reduced electronic coupling tenfold, confirming the critical role of dehydration and hydrophobic contacts in complex formation. These findings demonstrate that hydrophobic interactions facilitate the reorientation of Cyt *c* on C*c*O required for ET-active complex formation. Our results support a model in which Cyt *c* initially binds C*c*O in an ES complex stabilized by hydrophobic and electrostatic interactions. ET does not occur in this state due to the long Fe–Cu_A distance (~23 Å). Instead, thermal fluctuations drive a conformational transition to an ET-active complex with a shorter ET distance, enabling rapid ET. This transition, rather than ET itself, constitutes the rate-limiting step of the overall reaction. The proposed conformational gating mechanism underscores the importance of protein dynamics in regulating ET efficiency and coupling electron flow to proton pumping. By modulating ET rates through structural rearrangements, the system achieves optimal energy conversion rather than maximal electron flux, consistent with physiological requirements for maintaining proton/electron stoichiometry. The conformational gating mechanism in the Cyt *c*–C*c*O system highlights a general principle in biological ET: transient, energetically less stable conformations often mediate functionally critical steps. This dynamic regulation ensures synchronization between ET and proton pumping, preventing uncoupling that could compromise ATP synthesis.

REFERENCES

1. Sato, W., et al., (2026) *J. Phys. Chem. B.*, in press
2. Sato, W., et al., (2016) *J. Biol. Chem.*, *291*, 15320 – 15331

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Proton-coupled electron-transfer reduction of a quadruply-fused porphyrin derivative possessing imino-nitrogens at the periphery

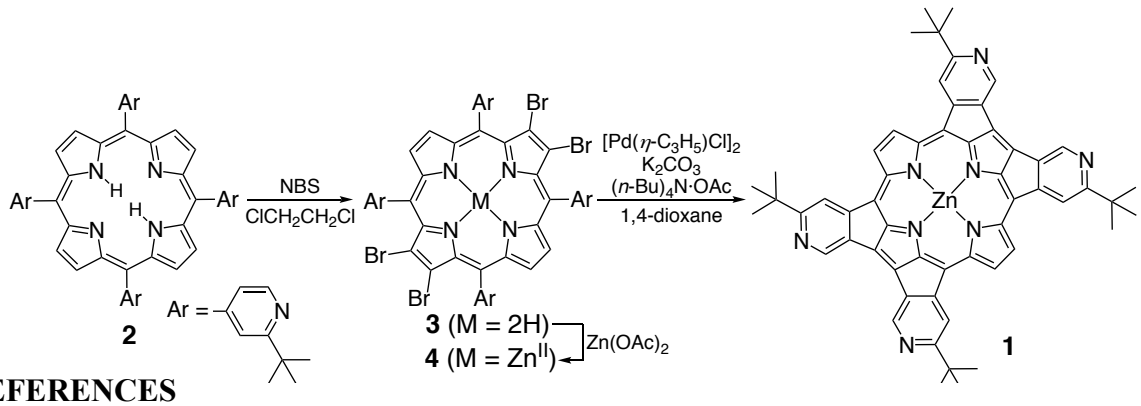
Tomoya Ishizuka[a], Yuma Obata[a], Risa Nishida[a], Takahiko Kojima[a]

[a]*Department of Chemistry, Faculty of Pure and Applied Sciences, University of Tsukuba*

ORALS

In recent years, research on the introduction of heteroatoms such as nitrogen at the periphery of aromatic rings has attracted considerable attention due to interest in the electron-acceptability [1, 2]. We reported the synthesis of a quadruply-fused porphyrin (QFP), in which aryl groups at the *meso*-positions and the pyrrole β-positions are covalently fused, using a Pd catalyst and this ring fusion proceeds regardless of the aryl groups [3]. Herein, four nitrogen atoms were introduced to the peripheral positions of a Zn^{II} complex of a QFP to obtain a tetraaza-derivative (**1**), containing four imino-nitrogens involved in the 30π aromatic circuit (Scheme). Addition of a strong acid such as triflic acid (TfOH) enables diprotonation of **1** and the diprotonated form of **1** shows a large positive shift of the first reduction potential. Furthermore, in the presence of excess TfOH, chemical or electrochemical reduction causes further protonation of the imino-nitrogen atoms of **1**, allowing further reduction of **1** through a proton-coupled electron-transfer mechanism. Based on DFT calculations, we have found that this phenomenon is caused by a large change in the pK_a of the outer imine nitrogens before and after the 1e⁻-reduction. Consequently, **1** allowed us to observe tetraprotonation and 4e⁻-reduction at a relatively positive potential to form $H_4\mathbf{1}^0$. $H_4\mathbf{1}^0$, obtained by 4e⁻-reduction of 30π-aromatic **1**, has been elucidated to exhibit 34π aromaticity, despite the fact that it is unable to draw an aromatic circuit with alternating single and double bonds. In this presentation, we will discuss on the aromaticity of $H_4\mathbf{1}^0$ in detail based on the ^{1}H NMR spectroscopy, NICS and ACID calculations.

Scheme. Synthesis of tetraaza-QFP derivative, **1**.



REFERENCES

1. E. Jin *et al.*, *J. Am. Chem. Soc.* **2021**, *143*, 10403.
2. T. Sakurai *et al.*, *Org. Lett.* **2021**, *23*, 2099.
3. T. Ishizuka *et al.*, *Chem. Commun.* **2013**, *49*, 5939

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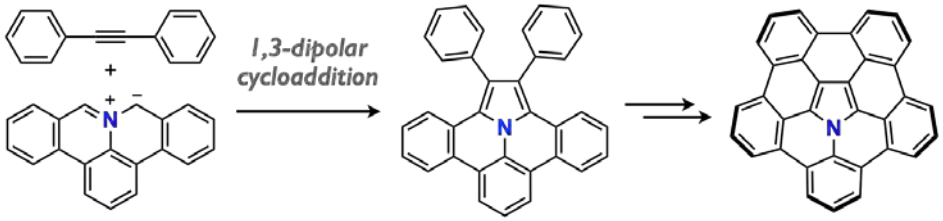


Azananographenes with Heptagonal or Octagonal Rings

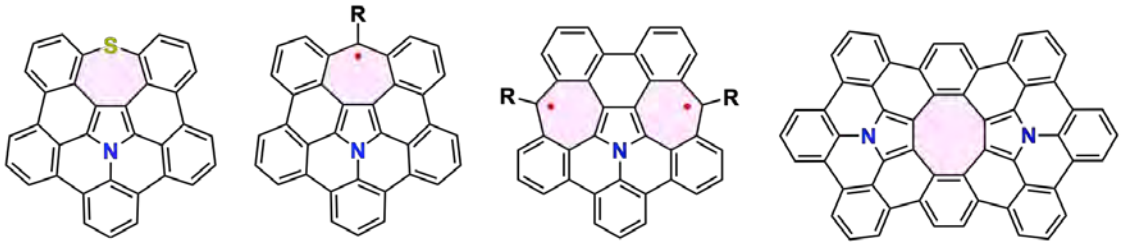
Shingo Ito[a]

[a]*School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University*

Our research group has been engaged in the development of novel π-functional molecules featuring unique structures and innovative properties. To date, we have employed 1,3-dipolar cycloaddition reactions of polycyclic aromatic azomethine ylides with various dipolarophiles to synthesize a wide range of nitrogen-embedded polycyclic aromatic molecules, including π-extended azacorannulenes.[1]



More recently, we have focused our efforts on heptagon- and octagon-embedded polycyclic aromatic molecules, which exhibit even more intriguing properties and potential applications. By applying our 1,3-dipolar cycloaddition strategy, we have successfully synthesized nitrogen-embedded polycyclic aromatic molecules fused with seven-membered rings[2–4] and eight-membered rings[5] (shown below). In this lecture, the synthesis, structures, properties, and potential applications of these molecules will be discussed in detail.



REFERENCES

1. S. Ito, Y. Tokimaru, K. Nozaki, Benzene-fused azacorannulene bearing an internal nitrogen atom. *Angew. Chem. Int. Ed.* **2015**, *54*, 7256.
2. W. Wang, F. Hanindita, Y. Tanaka, K. Ochiai, H. Sato, Y. Li, T. Yasuda, S. Ito, π-Extended pyrrole-fused heteropine: Synthesis, properties, and application in organic field-effect transistors. *Angew. Chem. Int. Ed.* **2023**, *62*, e202218176.
3. Y. Hamamoto, K. Ochiai, Y. Li, E. Tapavicza, S. Ito, Synthesis and properties of azahomocorannulenyl cations and radicals. *Angew. Chem. Int. Ed.* **2024**, *63*, e202319022.
4. Y. Hamamoto, W. Wang, Y. Li, S. Ito, Azadihomocorannulene as a heptagon-embedded diradicaloid. *Angew. Chem. Int. Ed.* **2025**, *64*, e202416654.
5. K. Nakamura, Q.-Q. Li, O. Krejčí, A. S. Foster, K. Sun, S. Kawai, S. Ito, On-surface synthesis of a π-extended diaza[8]circulene. *J. Am. Chem. Soc.* **2020**, *142*, 11363.

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De novo heme catalysts: a-helical coiled-coils with unprecedented heme&Trp redox cofactors for bioinspired catalysis featuring [Fe(IV)=O Por$^{\bullet+}$] and [Fe(IV)=O Trp$^{\bullet}$] catalytic intermediates.

Anabella Ivancich[a], Angela S. Gehrckens[a], Joseph Phillips[b], Iago De Assis Modenez[c], Stéphane Grimaldi[a], Guillaume Gerbaud[a], Stéphane Canaan[a], Barbara Schoepp-Cothenet[a], Piotr Mak[d], Anna F. Peacock[b], Vincent L. Pecoraro[c].

[a] *Research Unit UMR 7281, CNRS & Aix-Marseille University, Marseille. FRANCE.*
[b] *School of Chemistry, University of Birmingham. Edgbaston, United Kingdom (UK).*
[b] *Department of Chemistry. University of Michigan, Ann Arbor. USA.*
[b] *Department of Chemistry, Saint Louis University, St. Louis, Missouri, USA.*

In metalloproteins, transition metals are responsible for the redox reactions inherent to their catalytic function, which can be enhanced by concerted metal-radical chemistry. Heme-containing proteins are versatile catalysts performing disproportionation of H_2O_2 (catalases[1]), oxidation and haloperoxidation of organic substrates (monofunctional heme peroxidases[2], bi-functional catalase-peroxidases[1]) to oxygenation reactions (cyt P450 monooxygenases and NO synthases[2]). Such versatility relies on their heme axial ligands (Tyr, His, or Cys) and 2nd coordination spheres. The [Fe(IV)=O Por$^{\bullet+}$] catalytic intermediate shows concerted reactivity with specific Trp/Tyr sites. The [Fe(IV)=O Trp$^{\bullet}$] and/or [Fe(IV)=O Tyr$^{\bullet}$] species identified in mono and bi-functional peroxidases/KatGs and catalases allow accomplishing alternative reactions such as anti-tuberculosis prodrug activation in KatGs [3a, b], biomass bioconversion by lignin peroxidases [3c], oxidation of surface-binding substrates via long-range intramolecular electron transfer by cyt c peroxidase [3d] and lactoperoxidase [3e], and formate oxidation by *H. pylori* catalase [3f]. By exploiting de novo metalloprotein design, we have obtained a synthetic protein with a heme cofactor that can coordinate to either His or Cys, depending on pH, mimicking peroxidases or P450s, respectively, all in a single artificial metalloprotein [4a, b]. Modifying the proximal and distal sides of the His or Cys-coordinated heme allows us to address questions in natural P450 enzymes, as well as introducing tailored sites to stabilize a Trp$^{\bullet}$ formed subsequently to the [FeIV=O Por$^{\bullet+}$] intermediate, mimicking the protein-based radical chemistry of natural enzymes.

REFERENCES

1. A. Ivancich, P.C. Loewen. Encyclopedia of Biophysics, **2018**, Ed. Roberts, G. and Watts A., Springer.
2. T. L. Poulos, Chem. Rev. **2014**, 114, 3919-3962.
3. (a) R. Singh, J. Switala, P. C. Loewen, A. Ivancich *J. Am. Chem. Soc.* **2007**, 129, 15954-15963. (b) J. Colin, B. Wiseman, J. Switala, P. C. Loewen, A. Ivancich. J. Am. Chem. Soc. **2009**, 131, 8557-8563. (c) A.T. Smith, W. A. Doyle, P. Dorlet, A. Ivancich *Proc. Natl. Acad. Sci. USA* **2009**, 106, 16084-16089. (c) K. D. Miner, T. D. Pfister, P. Hosseinzadeh, N. Karaduman, L. J. Donald, P.C. Loewen, Y. Lu, A. Ivancich. *Biochemistry* **2014**, 53, 3781-3789. (d) P. J. Mak, S. Acebes, V. Guallar, J. R. Kincaid, A. Ivancich *J. Inorg. Biochem.* **2026**, 277, 113199.
4. (a) K. Koebke, T. Kühl, E. Lojou, B. Demeler, B. Schoepp-Cothenet, O. Iranzo, V. L. Pecoraro, A. Ivancich, *Angew. Chem. Int. Ed*., **2021**, 60, 3974-3978. (b) I. A. Modenez, A. Ivancich, V. L. Pecoraro. *Methods Enzymol. (Artificial Metalloproteins)* 2025, 720, 115-139

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Silicon(IV) porphyrazines and corrolazines

Svetlana Ivanova, Ekaterina Rychikhina, Pavel Stuzhin

Research Institute of Macroheterocycles, Ivanovo State University of Chemistry and Technology, 153000 Ivanovo, Russian Federation, svseriva@gmail.com

In the last decade, there has been increased interest in the study of silicon(IV) phthalocyanine (L_2SiPc) derivatives. Their solubility and ability to bind biomolecules can be tuned by varying the axial ligands L at the central silicon atom, while modification of the phthalocyanine macrocycle by substitution in benzene rings allows for changes in spectral and redox properties [1]. Contraction of the macrocycle leading to tetrabenzocorrolazines (LSiTBCzs), which are phthalocyanine analogues lacking one of the meso nitrogen atoms, can even enhance some potentially useful photochemical and photophysical properties [2].
In this work, silicon complexes with β-octaaryl substituted porphyrazines (L_2SiPz) and corrolazines (LSiCz) [3] and their derivatives with annulated pyrazine (Pyz) fragments are prepared (Figure 1). A comparative evaluation of the complexation and template cyclotetramerization methods for the preparation of Si(IV) porphyrazines is carried out. During the synthesis of $(HO)_2SiPzPh_8$, in addition to the target compound, an unusual complex with a tetraazachlorin-type macrocycle is formed, the structure of which was resolved by X-ray diffraction (Figure 2, axial ligands are not shown) [4]. The formation of the corresponding corrolazine structure occurs in boiling pyridine under the action of trichlorosilane on H_2PzPyz_4 or tri-alkyl/aryl-chlorosilane on appropriate silicon porphyrazine in the presence of Mg. The influence of axial substitution at the Si(IV) atom, as well as contraction of the macrocyclic ligand and benzo- and pyrazine-annulation on the spectral, photochemical, electrochemical and acid-base properties of the obtained silicon complexes is discussed.

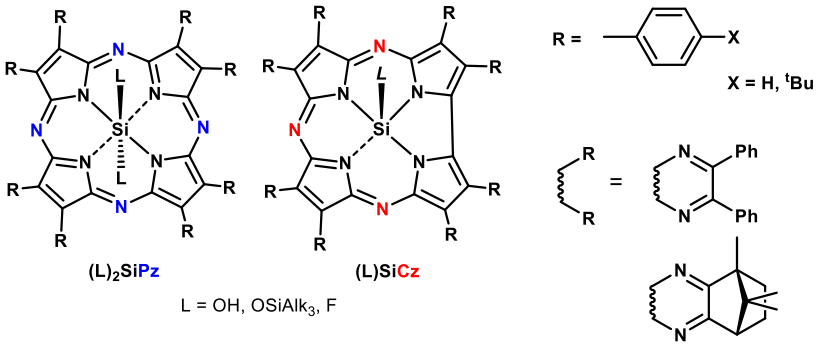


Figure 1.



Figure 2.

The work was supported by the RSF (grant No. 25-23-01389).

REFERENCES

1. K. Mitra, M.C.T. Hartman, *Org. Biomol. Chem*., **2021**, *19*, 1168.
2. Zhang X.-F. *Coord. Chem. Rev*. **2015**, *285*, 52.
3. Rychikhina E.D., Ivanova S.S., Novakova V., Stuzhin P.A. *Dalton Trans.* **2023**, *52*, 6831.
4. Rychikhina E.D., Ivanova S.S., Somov N., Lazovskiy D., Stuzhin P.A. *Dalton Trans.* **2025**, *54*, 11822.

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Secondary-Sphere-Controlled Metalloporphyrins for Activation of Small Molecules of Energy, Environmental, and Biological Relevance

Ivana Ivanovic-Burmazovic[a]

[a]*Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstr. 5-13, 81377 München, Germany*

ORALS

In this contribution, we present a comprehensive study on the modulation of catalytic reactivity of highly charged metalloporphyrins through systematic engineering of their secondary coordination sphere.

We have synthesized and fully characterized a modular library of more than twenty novel metalloporphyrins (predominantly iron, manganese, and cobalt), in which the number and spatial arrangement of crown ethers and positively charged functional groups were precisely varied. This rare-earth-free design strategy affords a highly adaptable family of catalytically active complexes capable of (i) photo- and electrocatalytic CO_2 reduction, extending selectively to methane formation, (ii) efficient catalytic removal of H_2S, and (iii) superoxide dismutation. Notably, superoxide conversion proceeds both via the classical pathway yielding O_2 and H_2O_2 and through an unusual dismutation route producing harmless water and molecular oxygen.

Beyond their catalytic performance, these metalloporphyrins serve as versatile molecular tools to disentangle the effects of secondary-sphere charge and non-redox-active metal cations (Li^+, Na^+, K^+, Cs^+, Ca^{2+}) on reactivity. We demonstrate how electrostatic interactions influence reactions with anionic substrates through ion aggregation and local concentration effects, stabilization of anionic intermediates or transition states, and modulation of metalloporphyrin redox potentials. These combined effects provide direct control over redox-catalytic properties.

Overall, this contribution highlights secondary-sphere engineering as a powerful strategy to tune metalloporphyrin reactivity and selectivity, offering new insights and opportunities for sustainable catalysis at the interface of energy conversion, environmental remediation, and biological redox chemistry..

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Metal-Sulfur Cluster Catalysts for the Direct Conversion of CO_2 into CH_4

Hitoshi Izu[a], Yuto Matsuoka[a], Kodai Yamamoto[a], W. M. C. Sameera[b], Kazuki, Tanifuji[a], Yasuhiro Ohki[a]

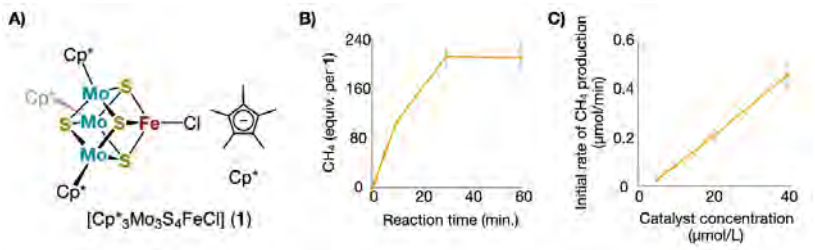
[a]*Institute for Chemical Research, Kyoto University*
[b]*Department of Space, Earth and Environment, Chalmers University of Technology*

ORALS

In nature, metal-sulfur clusters function as enzymatic active sites and catalyze the transformation of inert small molecules such as N_2 and CO_2 [1,2]. We have previously focused on the catalytic functions of such biological clusters and discovered that the synthetic cubane-type metal-sulfur cluster [$Cp^*_3Mo_3S_4FeCl$] (**1**; Cp^* = C_5Me_5, Figure A) promotes the silylation of N_2 [3]. In this cluster, the strongly bound Cp^* ligands on the Mo centers confine the reactive site to the Fe center, while combination with a cubane-type inorganic framework provides high structural stability. In the present study, we sought to exploit the stability of cluster **1** and apply it to CO_2 reduction reactions mediated by metal-sulfur clusters, as previously reported [4]. As a result, cluster **1** exhibited an exceptionally high catalytic turnover number (TON) for the direct reduction of CO_2 to CH_4 and displayed reactivity distinct from that of conventional homogeneous catalysts.

Under an atmosphere of CO_2 (1 atm), treatment of cluster **1** with chemical reductant (5000 equiv) and H_2O as a proton source afforded CH_4 in 230 ± 18 equivalents relative to the cluster, corresponding to a reductant efficiency of 37% (Figure B). The formation of H_2 was also observed, with a yield of 1396 ± 48 equivalents and a reductant efficiency of 56%. Because the reaction was presumed to terminate due to consumption of the reductant, the amount of reductant was increased. Under these conditions, the TON for CH_4 formation reached a maximum value of 127000 ± 5000, representing the highest value reported to date among homogeneous catalysts. Notably, formation of CO, a common product in CO_2 reduction, was strongly suppressed and remained below 0.3% based on reductant efficiency.

To gain insight into the nature of the catalytically active species, the initial rate of CH_4 formation was plotted as a function of cluster concentration. A linear relationship was observed (Figure C), suggesting that cluster **1** operates as a molecular catalyst for the conversion of CO_2 to CH_4. In this presentation, we further discuss the mechanism of CH_4 formation and the origin of the unique reactivity of cluster **1**, based on stoichiometric reactions and intermediate-trapping experiments.



REFERENCES

1. T. Spatzal, M. Aksoyoglu, L. Zhang, S. L. A. Andrade, E. Schleicher, S. Weber, D. C. Rees, O. Einsle, *Science* **2011**, *334*, 940.
2. J. Fesseler, J.-H. Jeoung, H. Dobbek, *Angew. Chem. Int. Ed*. **2015**, *54*, 8560.
3. Y. Ohki, K. Munakata, Y. Matsuoka, R. Hara, M. Kachi, K. Uchida, M. Tada, R. E. Cramer, W. M. C. Sameera, T. Takayama, Y. Sakai, S. Kuriyama, Y. Nishibayashi, K. Tanifuji, *Nature* **2022**, *607*, 86.
4. For example, see: K. Tanifuji, N. Sickerman, C. C. Lee, T. Nagasawa, K. Miyazaki, Y. Ohki, K. Tatsumi, Y. Hu, M. W. Ribbe, *Angew. Chem. Int. Ed*. **2016**, *55*, 15633.

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Functional applications of triazole-bearing porphyrin derivatives

Woo-Dong Jang

Yonsei University. 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Korea

ORALS

Porphyrins are a class of aromatic macrocycles composed of four pyrrole subunits connected via methine bridges. Owing to their extended π-conjugation, porphyrins exhibit distinct photophysical and electrochemical properties. The four nitrogen atoms in the porphyrin core can chelate various metal ions, allowing fine-tuning of their physical and chemical properties through metal coordination. In addition, the highly symmetric architecture of porphyrins makes them attractive building blocks for the construction of functional supramolecular architectures.

Inspired by the diverse roles of porphyrins and chlorophylls in biological systems, including oxygen transport, enzymatic catalysis, and light harvesting, we have recently designed a series of porphyrin-based bio-inspired functional materials. In particular, we have focused on triazole-functionalized porphyrins, in which triazole units are introduced as versatile recognition and coordination motifs. The triazole moiety provides directional hydrogen-bonding capabilities and additional metal-binding sites, thereby enabling cooperative interactions with guest species.

Using these triazole-decorated porphyrin scaffolds, we have developed several types of receptor molecules that selectively bind anionic and cationic species. By combining metalloporphyrin cores with triazole-based hydrogen-bonding motifs or secondary coordination sites, we achieved enhanced sensitivity and selectivity in chemosensing applications. These systems serve as biomimetic models that emulate key features of natural porphyrin-based active sites. The detailed design principles and functional properties of our triazole-containing porphyrin receptors will be presented in this symposium.

REFERENCES

1. D. Yim, J. Sung, S. Kim, J. Oh, H. Yoon, Y. M. Sung, D. Kim, W.-Do. Jang, *J. Am. Chem. Soc.*, **2017**, 139(2), 993 - 1002.
2. J. Oh, H. Yoon, Y. M. Sung, P. Kang, M.-G. Choi, W.-D. Jang, D. Kim, *J. Phys. Chem. B*, **2015**, 119(23), 7053 - 7061.
3. H. Kim, K.-I. Hong, J. H. Lee, P. Kang, M.-G. Choi, W.-D. Jang *Chem. Commun.*, **2018**, 54(77), 10863 - 10865.

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Augmenting DNA Nanotechnology using Synthetic Macrocycles

Janarthanan Jayawickramarajah[a]*, Soumen Pradhan[a], Aunindya Jyoti[a],

[a] *Department of Chemistry, Southern Methodist University, Dallas, USA*

The development of controllable molecular and nano-machines that operate in aqueous and biological environments is an important endeavor, with potential practical applications in biosensing, theranostics, and computing. Regarding well-controlled systems and assemblies that work in water, DNA nanotechnology has been leading due to the programmability of DNA structures governed by simple base-pairing rules. In this talk, we explain how strategic covalent attachment of various macrocycles, such as porphyrins, cyclodextrins, and cucurbiturils, to DNA can improve DNA nanotechnology by creating novel systems with potential photonic, therapeutic, and diagnostic applications. This talk also explores new directions in developing mechanically interlocked (bio) polymers.

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Metal Complexes of Modified Corroles as Novel Electronic Materials

Jeyaraman Sankar,[a*] Baranya Kanungo[a] and Senthamizh Selven[a]

[a]*Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal, India - 462066*

ORALS

Renewed interest in metalloporphyrins as new generation electronic materials is gaining traction recently due to their multifunctional nature.[1] While metallocorroles inherit many of the advantages of metalloporphyrins, they retain their unique electronic structure, thereby exhibiting distinct optoelectronic and redox properties. In this regard, suitable functionalization of corroles can be explored to bind metal ions in a manner similar to that of porphyrins, but preserving their own electronic characteristics. This strategy would result in a molecular platform that behaves like porphyrins for metal binding while simultaneously maintaining the (electronic) structure of corroles. Towards this end, core-modified corroles have been interesting examples in which the metal ions are present in their dicationic form[2,3]. In this regard, our group has recently developed a few interesting examples of metal complexes of core-modified corroles. In this lecture, their optical properties, redox characteristics, and magnetic properties will be discussed in detail.

REFERENCES

1. Ranieri , D.; Santanni , F.; Privitera , A.; Albino , A.; Salvadori, E.; Chiesa, M.; Totti, F.; Sorace, L.; Sessoli, R. *Chem. Sci*., **2022**, *14*, 61.
2. Orlowski, R. ; Gryko D. ; Gryko, D. T. *Chem. Rev*. **2017**, *117*, 4, 3102.
3. Sankar, J. ; Rath, H. ; Prabhuraja, V. ; Gokulnath, S. ; Chandrashekar, T. K. ; Purohit, C.S. ; Verma, S. *Chem. Eur. J*. **2007**, *13*, 105.

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Electrosynthesis of Verdoheme and Biliverdin Derivatives Following Enzymatic Pathways

Jianbing "Jimmy" Jiang

University of Cincinnati, USA

Artificial syntheses of biologically active molecules have been fruitful in many bioinspired catalysis applications. Specifically, verdoheme and biliverdin, bearing polypyrrole frameworks, have inspired catalyst designs to address energy and environmental challenges. Despite remarkable progress in benchtop synthesis of verdoheme and biliverdin derivatives, all reported syntheses, starting from metalloporphyrins or inaccessible biliverdin precursors, require multiple steps to achieve the final desired products. Additionally, such synthetic procedures use multiple reactants/redox agents and involve multistep purification/extraction processes that often lower the yield. However, in a single step using atmospheric oxygen, heme oxygenases selectively generate verdoheme or biliverdin from heme. Motivated by such enzymatic pathways, we report a single-step electrosynthesis of verdoheme or biliverdin derivatives from their corresponding meso-aryl-substituted metalloporphyrin precursors.[1] Our electrosynthetic methods have produced a copper-coordinating verdoheme analog in >80% yield at an applied potential of 0.65 V vs ferrocene/ferrocenium in air-exposed acetonitrile solution with a suitable electrolyte. These electrosynthetic routes reached a maximum product yield within 8 h of electrolysis at room temperature. The major products of verdoheme and biliverdin derivatives were isolated, purified, and characterized using electrospray mass spectrometry, absorption spectroscopy, cyclic voltammetry, and nuclear magnetic resonance spectroscopy techniques. Furthermore, X-ray crystallographic data were collected for select cobalt (Co)- and Cu-chelating verdoheme and metal-free biliverdin products. Electrosynthesis routes for the selective modification at the macrocycle ring in a single step are not known yet, and therefore, we believe that this report would advance the scopes of electrosynthesis strategies.
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REFERENCES

1. J. Am. Chem. Soc. 2024, 146, 15955–15964. DOI: 10.1021/jacs.4c02847

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Ångström-Scale Insights into On-Surface Porphyrin Chemistry via Tip-Enhanced Raman Spectroscopy

Nan Jiang[a,b]

[a]*Department of Chemistry, University of Illinois Chicago, Chicago, IL 60607, USA*
[b]*Department of Physics, University of Illinois Chicago, Chicago, IL 60607, USA*

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Our research investigates how local environments influence single-molecule and nanostructure properties on surfaces with Ångström-scale resolution. Tip-Enhanced Raman Spectroscopy (TERS) combines the spatial resolution of Scanning Tunneling Microscopy (STM) with the chemical sensitivity of Raman spectroscopy. By utilizing a plasmonically active scanning probe, the Raman signal at the tip-sample junction is greatly enhanced, enabling single-molecule probing. This method, further aided by the benefits of ultrahigh vacuum, is uniquely capable of controlling localized plasmons via an atomistic approach. We are able to obtain (i) single-molecule chemical identification;[1] (ii) quantum characterization of adsorbate-substrate interactions at the single chemical bond level; [2-5] (iii) atomic-scale insights into the reactivity on surfaces; [6, 7] By investigating single porphyrin molecules, superstructures, and the adsorption orientations obtained from the vibrational modes, we extract novel surface information at an unprecedented spatial (< 1 nm) and energy (< 10 wavenumber) resolution. Another application of localized surface plasmons is to achieve site-selective chemical reactions at sub-molecular scale. We recently selectively and precisely activated multiple chemically equivalent reactive sites one by one within the structure of a single porphyrin molecule by scanning probe microscopy tip-controlled plasmonic resonance.[8] Our method can interrogate the mechanisms of forming and breaking chemical bonds at the Ångström scale in various local environments, which is critical in designing new atom- and energy-efficient materials and molecular assemblies with tailored physical and chemical properties. Overall, our work provides unprecedented Ångström-scale insights into the chemical behavior, reactivity, and plasmon-mediated transformations of porphyrin molecules on surfaces, revealing fundamental structure–function relationships at the single-molecule level.

REFERENCES

1. *Nano Letters*, 19, 3267-3272 (2019).
2. *ACS Nano*, 18, 32118-32125 (2024).
3. *ACS Nano*, 19, 15363-15370 (2025).
4. *Chem*, 11, 202290 (2025).
5. *Journal of Physics: Condensed Matter*, 34, 204008 (2022).
6. *Nature Communications*, 13, 1796 (1-9) (2022).
7. *Angewandte Chemie International Edition*, 62, e202306590 (2023).
8. *Journal of the American Chemical Society*, 144, 5, 2051-2055 (2022).

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Catalytic activation of CO_2 via photonic and molecular design

Jieun Jung[a]

[a] *Department of Material and Life Science, Graduate School of Science, Nagoya University*

The catalytic activation of carbon dioxide (CO_2) remains a central challenge in molecular catalysis, as it requires precise control over multi-electron and multi-proton transfer processes. Molecular catalysts offer well-defined platforms to elucidate reaction pathways and establish design principles for efficient CO_2 conversion. For effective utilization of solar energy, particularly within the visible-light region, catalytic systems to harvest longer-wavelength light are highly desirable. Our group has been developing robust tetradentate PNNP-type metal complexes[1] such as (PNNP)Ir and (PNNP)Ru for photocatalytic CO_2 reduction. These ligands consist of a bipyridine backbone and two organophosphorus groups, which allow tuning of electronic and steric properties through ligand modification. However, these complexes typically exhibit weak absorption in the visible-light region, limiting their activity to short-wavelength irradiation. Herein, we report a (PNNP)Os complex as a panchromatic, self-photosensitized catalyst for CO_2 reduction, capable of utilizing a broad range of visible light. The Os complex displays strong absorption across the visible region and promotes photocatalytic CO_2 reduction (Figure 1).

Upon photoirradiation ($\lambda \geq 400$ nm) of a CO_2-saturated mixture of DMA/H_2O/TEOA containing the photocatalyst, (PNNP)Os (**1**) and a sacrificial electron donor, 1,3-dimethyl-2-phenyl-2,3-dihydro-1*H*-benzo[*d*]imidazole (BIH), selective formation of carbon monoxide (CO) as the main product was observed without the need for an additional photosensitizer. Product yields increased with prolonged irradiation, reaching a total turnover number (TON) of 625 over 144 h. Notably, photocatalytic reduction of CO_2 also proceeded under monochromatic lights such as blue- (λ_0 = 405 nm), green- (λ_0 = 525 nm), or red- (λ_0 = 630 nm) light, affording TON_{CO} values of 187, 86, and 47, respectively in 48 h. It is noteworthy that replacing the metal center in the PNNP ligand from Ir to its neighboring element Os shifted the primary product from HCO_2H to CO.

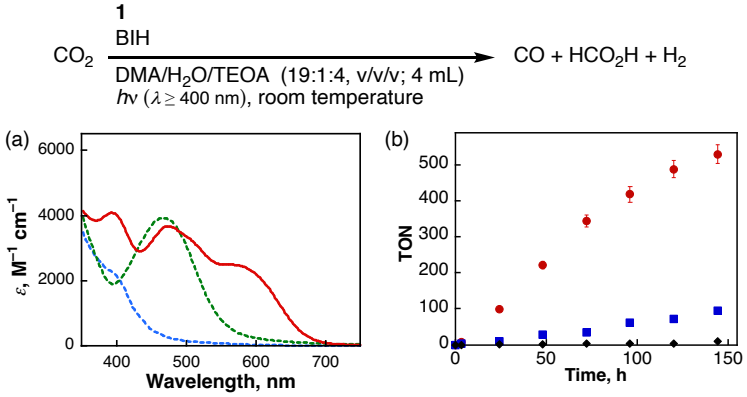


Figure 1. (a) UV-vis absorption spectrum of **1** (red), (PNNP)Ru (green), and (PNNP)Ir (blue) complexes in a deaerated DMA solution. (b) Time course plots of products [CO (red), HCO_2H (blue), and H_2 (black)] produced in the photocatalytic reduction of CO_2 in a CO_2-saturated mixture of DMA/H_2O/TEOA (19:1:4, v/v/v) containing a catalytic amount of **1** (20 μM) and BIH (0.1 M) at 298 K under photoirradiation.

REFERENCES

1. (a) Kamada, K. ; Jung, J.; Wakabayashi, T.; Sekizawa, K.; Sato, S.; Morikawa, T.; Fukuzumi, S.; Saito, S. *J. Am. Chem. Soc.* **2020**, *142*, 10261. (b) Kamada, K.; Jung, J.; Kametani, Y.; Wakabayashi, T.; Shiota, Y.; Yoshizawa, K.; Bae, S. H.; Muraki, M.; Naruto, M.; Sekizawa, K.; Sato, S.; Morikawa, T.; Saito, S. *Chem. Commun*. **2022**, *58*, 9218. (c) Kamada, K.; Okuwa, H.; Wakabayashi, T.; Sekizawa, K.; Sato, S.; Morikawa, T.; Jung, J.; Saito, S. *Synlett* **2022**, *33*, 1137.

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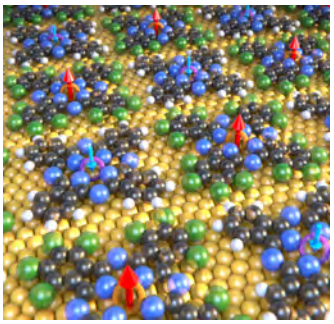
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A surface scientist's view into the key mechanisms of porphyrins and phthalocyanines and their chemical, electronic and spin-tronic action in a broad range of applications

J . Girovsky[1], M. Baljozovic[1], S. Nowakowska[2], J. Nowakowski[1], A. Wäckerlin[2], S.F. Mousavi[2], C. Wäckerlin[1], A. Ahsan[2], J. Dreiser[1], J. Lobo Checa[1, 2], M. Stöhr[2], L. H. Gade[3], S. Decurtins[4], S-X. Liu[4], P. M. Oppeneer[5], K. Tarafder[5], N. Ballav[6], and T. A. Jung[1,2]

[1] Paul Scherrer Institute, Switzerland; [2] University of Basel, Switzerland; [3] Heidelberg University, Germany; [4] University of Bern, Switzerland; [5] Uppsala University, Sweden; [6] Indian Institute of Science Education and Research, India



In our work, we investigate porphyrin-based on-surface architectures which exhibit extraordinary properties, e.g. electronic, magnetic and quantum properties originating from the reduced dimensionality and the atomically precise self-assembled architectures. Both unconventional H-bonding [1] and direct site-specific interaction [2] of the porphyrin's central metal with the substrate direct the assemblies. We look at the coordination chemistry and magneto-chemistry down to the scale of individual molecules by combining scanning probe microscopy/spectroscopy, photoelectron and photo-absorption spectroscopy and density functional theory. Complex electronic [3] and magnetic [4] phases arise from the 2D periodic lattice interacting with substrate electronic states. Furthermore, sub-lattices in 2D 'checkerboard' architectures of magnetic molecules on magnetic substrates can be selectively switched by chemical ligation [5]. Notably, we observed the first example of 2D ferrimagnetic long-range order and remanence for such a 2D architecture on non-magnetic Au(111) [4]. Uniquely, specifically engineered on-surface architectures contribute to our understanding of fundamental interactions in host-guest systems and enable the operation of quantum states with partial delocalization across the supramolecular on-surface architecture [5]. In our quest to improve these systems and develop new ones, we are unraveling more and more of the on-surface chemistry [6] required to engineer low-dimensional materials with unprecedented properties by controlling their architecture. In particular, this involves on-surface supramolecular, - coordination and – magneto-chemistry.

REFERENCES

[1] Mousavi, S. F. et al., Commun. Chem. (2025), https://doi.org/10.1038/s42004-025-01607-x
[2] A. Waeckerlin et al., Nano Lett. 2017, 17, 1956−1962
[3] Lobo-Checa, J. et al., Science 325:300 (2009)
[4] Girovsky, J. et al., Nat. Commun., DOI: 10.1038/ncomms15388 (2017).
[5] C. Waeckerlin et al, 10.1002/adma.201204274
[5] Nowakowska, S. et al., 10.1021/acsnano.7b07989
[6] Ballav N., et al., JPCL 4:2303 (2013) [4].

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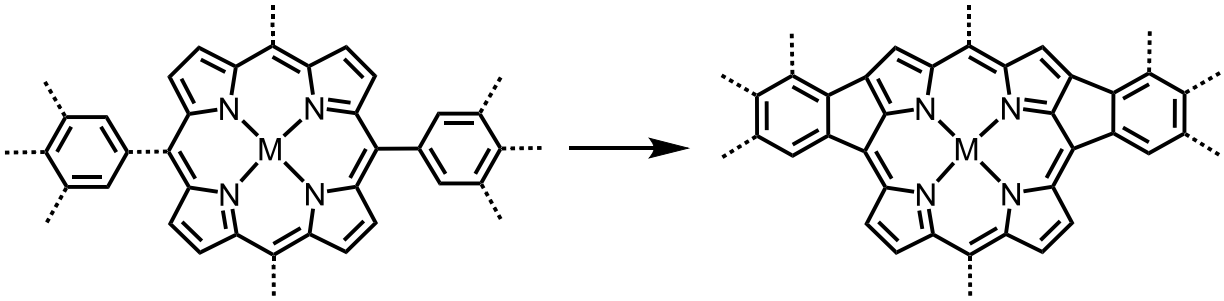


Fusing porphyrins to PAHs

Norbert Jux[a], **Christoph Oleszak**[a]

[a] *Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Chemistry & Pharmacy and Interdisciplinary Center for Molecular Materials. Erlangen, Germany.*

Fusing porphyrins to various polycyclic aromatic hydrocarbons is an excellent strategy to expand the π-system of the porphyrin and add functionality.[1-2] Thus, new chromophores are obtained which possess, among other interesting qualities, red-shifted UV/vis absorptions.



We present our approach to π-extended fused porphyrins via Scholl oxidation of meso-positioned aryl groups to the core.[3, 4]

REFERENCES

1. Roznyatovskiy VV, Leeb CH and Sessler JL. *Chem. Soc. Rev.* 2013; **42**: 1921-1933.
2. Lewtak JP and Gryko, DT. *Chem. Commun.* 2012; **48**: 10069-10086.
3. Martin MM, Oleszak C, Hampel F and, Jux N. *Eur. J. Org. Chem.* 2020; **40**: 6578-6762.
4. Oleszak C, Schol PR, Ritterhoff, CL, Krug M, Martin MM, Yo B, Meyer B, Clark T, Guldi, DM and Jux N. *Angew. Chem. Int. Ed.* 2024; **63**: e202409363.

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Heme-M (M = Cu or non-heme Fe) Modeling: Synthetic Constructs and O_2 or NO Reactivity

Kenneth D. Karlin[a]

[a]*Dept. Chemistry, Johns Hopkins University, Baltimore USA*

ORALS

Heme/copper oxidases (HCO's) such as cytochrome *c* oxidase (C*c*O) facilitates the $4e^-/4H^+$ reduction reductive cleavage of dioxygen to water, coupling this chemistry with mitochondrial membrane proton translocation; the proton gradient thus produced drives the synthesis of ATP, our cellular mobile energy currency [1]. Nitric Oxide Reductases (NOR's) are structurally related heme/non-heme iron enzymes, effecting the $2e^-/2H^+$ reduction of 2NO to N_2O (+ H_2O); these are related in evolution to HCO's [2]. It has been recently revealed that there exist NOD's (Nitric Oxide Dismutases; NOD's; 2NO –> N_2 + O_2) which account for anaerobic organism (i.e., bacteria, archaea) generation of "dark oxygen"; these NOD enzymes are related to qNOR's (NOR's with a quinol electron source/carrier), but they possess a somewhat altered heme/non-heme iron active site [3-4]. Our research aims to contribute to a fundamental understanding of O_2 and/or NO reactivity at such heme/Cu and/or heme/non-heme iron (heme/Fe_B) centers via the examination of synthetically derived chemical model systems [1]. The O_2 or NO reduction-protonation steps do not exhibit the same behavior as in pure aqueous media, because O_2/NO reduced/protonated derivatives are metal-ion bound. In this lecture, we will emphasize the description of relevant chemistry of O_2 and NO with heme-copper assemblies. Synthetically designed and constructed reduced (heme)Fe^{II}-Cu^{I}(ligand) ensembles are described; their reactions with O_2 give variable high-spin (iron) peroxo-bridged Fe^{III}-(m-O_2^{2-})-Cu^{II}(ligand) complexes. Conversion to low-spin analogues occurs by addition of a heme axial-ligand (B) giving (B)Fe^{III}-(m-O_2^{2-})-Cu^{II}(ligand) peroxo species The nature of the Cu- and Fe- peroxo-ligation of dictates the structural/physical properties and subsequent reactivity of these assemblies; our investigations employing varying proton and electron sources reveals that either metal-O bond cleavage leads to release of hydrogen peroxide, or biomimetic O–O reductive cleavage reactions take place [5]. Time permitting, aspects of the biochemistry of NOR's and NOD's will be described and model systems for NOR biomimetic reactivity may be presented.

REFERENCES

1. Adam, S. M.; Wijeratne, G. B.; Rogler, P. J.; Diaz, D. E.; Quist, D. A.; Liu, J. J.; Karlin, K. D. Synthetic Fe/Cu Complexes: Toward Understanding Heme-Copper Oxidase Structure and Function *Chem. Rev.* **2018**, *118*, 10840.
2. Lehnert, N.; Kim, E.; Dong, H. T.; Harland, J. B.; Hunt, A. P.; Manickas, E. C.; Oakley, K. M.; Pham, J.; Reed, G. C.; Alfaro, V. S. The Biologically Relevant Coordination Chemistry of Iron and Nitric Oxide: Electronic Structure and Reactivity. *Chem. Rev.* **2021**, *121*, 14682-14905.
3. Ruff, S. E.; Humez, P.; de Angelis, I. H.; Diao, M.; Nightingale, M.; Cho, S.; Connors, L.; Kuloyo, O. O.; Seltzer, A.; Bowman, S.; Wankel, S. D.; McClain, C. N.; Mayer, B.; Strous, M. Hydrogen and dark oxygen drive microbial productivity in diverse groundwater ecosystems. *Nature Commun.* **2023**, *14*, 3194.
4. Murali, R.; Pace, L. A.; Sanford, R. A.; Ward, L. M.; Lynes, M. M.; Hatzenpichler, R.; Lingappa, U. F.; Fischer, W. W.; Gennis, R. B.; Hemp, J. Diversity and evolution of nitric oxide reduction in bacteria and archaea. *Proc. Natl. Acad. Sci. U. S. A.* **2024**, *121*, e2316422121.
5. Adam, Suzanne M.; Garcia-Bosch, Isaac; Schaefer, Andrew W.; Sharma, Savita K.; Siegler, Maxime A; Solomon, Edward I.; Karlin, Kenneth D., "Critical Aspects of Heme–Peroxo–Cu Complex Structure and Nature of Proton Source Dictate Metal–O_{peroxo} Breakage versus Reductive O–O Cleavage Chemistry", *J. Am. Chem. Soc*. **2017**, *139*, 472.

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Tuning Photophysical Properties of Metalloporphyrins via Electronic Control: Experimental & Computational Insights

Malkanthi K. Karunananda*[a], Madhusha Manna Peruma[a], Rishi Ranjan[a], Dariusz M. Niedzwiedzki[b]

[a]*Department of Chemistry, Saint Louis University, St. Louis, MO, 63103, United States.*
[b]*Department of Biology, Washington University in St. Louis, St. Louis, MO, 63130, United States.*

Abstract. Photosensitizers that absorb photon energy and after excitation, participate in transfer of energy or electrons, are highly in demand due to their versatile applications in organic synthesis, light-emitting devices, solar fuel cells, artificial photosynthesis, and photodynamic therapies . Metalloporphyrins have emerged as a prominent class of photosensitizers due to their stability, tunability and enhanced photophysical properties. Here, a comprehensive experimental and computational study is presented where the electronics of a series of zinc dipyrrins were tuned to modulate their photophysical properties. The electronic excited state parameters of the complexes were investigated with time-resolved spectrosocpies as time-correlated-single-photon-counting and ultra-fast transient absorption. Fluorescence quantum yields were also obtained experimentally. Time-dependent density functional theory (TD-DFT) and natural bond order (NBO) calculations were performed to map out the natural transition orbitals (NTO) and molecular orbitals (MO) involved in the electronic transitions to analyze and understand the photophysical trends emerged from the experimental data. Insights gained from this study inform the development of novel photocatalytic synthetic methodologies and photodynamic therapies which will also be discussed.

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Overcoming drug delivery challenges in antimicrobial photodynamic therapy

Giulia Kassab[a], Juan Chen[a], Gang Zheng[a,b]

[a]*Princess Margaret Cancer Center, University Health Network, Toronto, ON, Canada;*
[b]*Department of Medical Biophysics, University of Toronto, Toronto, ON, Canada*

Antimicrobial photodynamic therapy (aPDT) is a promising approach to treating infections that combines a photosensitizer, light at a specific wavelength, and molecular oxygen, producing reactive oxygen species that lead to cell death. Unlike traditional antibiotic therapy, aPDT does not target a specific structure or molecule, thereby preventing the development of resistance. However, as it is not target-specific, selectivity in aPDT is achieved by localized delivery of light and the photosensitizer, and by using targeting agents. For the treatment of pneumonia, localized, pain-free respiratory delivery of PSs can be achieved via nebulization [1]. However, light absorption in the visible range limits effective tissue penetration. Another challenge for effective lung aPDT is that many PSs interact with endogenous lung surfactant (LS), reducing their availability to the bacterial target and leading to a loss of activity [2]. Therefore, the development of aPDT agents that can overcome the barrier of interaction with the LS would be essential for a successful aPDT treatment of pneumonia. Wound infections pose very different challenges. On one hand, they are often treated with topical, localized treatments due to their superficial nature. This enables the use of PSs activated by shorter wavelengths, which have limited applications in cancer research. However, chronic wound infections are often caused by multi-species biofilms, which are much more difficult to treat. In these infections, slow-growing, persistent biofilms induce chronic inflammation and oxidative damage, while also hindering the immune response [3]. Thus, effective aPDT treatments must penetrate the extracellular matrix of biofilms and completely eradicate a broad spectrum of infectious agents while preserving host tissue. Understanding how to circumvent these limitations has led to significant improvement of aPDT agents [4-5]. This presentation will show the recent advancements made in the aPDT of pneumonia and wound infections, including the rational design of photosensitizers, targeting agents, and nanodelivery systems; their impact on biological activity and selectivity against several bacterial and fungal pathogens; and how their different characteristics translate into different *in vitro* and *in vivo* disease models.

REFERENCES

1. G. Kassab *et al.*, “Nebulization as a tool for photosensitizer delivery to the respiratory tract,” *J. Biophotonics*, vol. 12, no. 4, p. e201800189, Apr. 2019, doi: 10.1002/jbio.201800189.
2. G. Kassab *et al.*, “Lung surfactant negatively affects the photodynamic inactivation of bacteria—in vitro and molecular dynamic simulation analyses,” *Proc. Natl. Acad. Sci.*, vol. 119, no. 25, p. e2123564119, Jun. 2022, doi: 10.1073/pnas.2123564119.
3. J. Hurlow and P. G. Bowler, “Acute and chronic wound infections: microbiological, immunological, clinical and therapeutic distinctions,” *J. Wound Care*, vol. 31, no. 5, pp. 436–445, 2022, doi: 10.12968/jowc.2022.31.5.436.
4. H. H. Buzzá *et al.*, “Porphyrin nanoemulsion for antimicrobial photodynamic therapy: effective delivery to inactivate biofilm-related infections,” *Proc. Natl. Acad. Sci.*, vol. 119, no. 46, pp. 1–9, Nov. 2022, doi: 10.1073/pnas.2216239119.
5. G. Kassab *et al.*, “Structural Effect of Rhenium- and Iridium-Complex Liposome Composition on Their Selectivity for Antimicrobial Photodynamic Therapy,” *Small Sci.*, vol. 4, no. 2, 2024, doi: 10.1002/smsc.202300131.

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On-Surface Syntheses of Extended Porphyrins via Cyclodehydrogenation and Homocoupling of Trifluoromethyl groups

Shigeki Kawai[a,b]

[a]*National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan*
[b]*University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan*

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On-surface chemical reactions have become a very powerful technique for synthesizing nanostructures by linking small molecules in a bottom-up approach. Porphyrin is one of the most attractive molecules due to its unique electronic and magnetic properties, which can be tuned by introducing a variety of metal cores or extending its structure. These properties also make porphyrin a highly attractive precursor molecule for on-surface reactions.

We present the on-surface synthesis of multi-block co-oligomers from trifluoromethyl (CF3) substituted porphyrin metal complexes. Oligomerization on Au(111) is demonstrated using a combination of bond-resolved scanning probe microscopy and density functional theory (DFT) calculations. Given that most reactants are simultaneously activated at certain temperatures, a controlled sequential reaction has remained challenging. We found that even after the first oligomerization of a single monomer unit, the oligomer's termini retain the CF_3 group, which can be used as a reactant for further coupling in a sequential manner. Consequently, copper, cobalt, and palladium complexes of bisanthracene-fused porphyrin oligomers were linked with each other in a designed order.

We also present the on-surface synthesis of phenalenyl-expanded Au porphyrin via cyclodehydrogenation, investigated using a combination of non-contact atomic force microscopy, scanning tunnelling microscopy, scanning tunnelling spectroscopy, and theoretical calculations. After annealing, we found two different products. Although the structures are nearly identical, the charge state significantly affected to the spin states. We found that the role of molecule-substate interactions and the resulting charge transfer in the gold complex tune the spin and electronic properties of the extended porphyrins.

REFERENCES

1. S. Kawai, A. Ishikawa, S. Ishida, T. Yamakado, Y. Ma, K. Sun, Y. Tateyama, R. Pawlak, E. Meyer, S. Saito, A. Osuka. Angew. Chem. Int. Ed. 2022, 61, e202114697
2. D. Li, M. Kumar, O. Stetsovych, B. Lowe, R. Sengupta, H. Hayashi, H. Maeda, P. Jelínek, S. Kawai (Submitted).

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Photodynamic Therapy Using Chlorin e6-Bearing Pullulan Nanogel as Nano-Based Photosensitizer

Riku Kawasaki[a], Takuro Eto,[a] Shoma Takeichi,[a] Naoki Tarutani,[a] Kiyofumi Tarutani,[a] Keita Yamana,[a] Takeshi Nagasaki,[b] Atsushi Ikeda[a]

[a]*Applied Chemistry Program, Graduate School of Advanced Science and Engineering, Hiroshima University*
[b]*Department of Applied Chemistry and Bioengineering, Graduate School of Engineering, Osaka Metropolitan University. Japan.*

With high tumor specificity, low invasiveness, high cure rate, and excellent *in situ* workability, photodynamic therapy (PDT) is one of the most elegant therapeutic modalities for cancer treatment. PDT is achieved through oxidative stress induced by reactive oxygen species (ROS) generated by photosensitizers upon light irradiation at an optimal wavelength. Porphyrins, chlorins, and phthalocyanines have been widely explored as photosensitizers due to their excellent photo-triggered activatability in the visible-to-near-infrared region, arising from their intense absorption bands, including the Soret band and Q bands. In particular, their Q-band absorption in the red-to-near-infrared region enables deeper tissue penetration of excitation light, making these chromophores highly suitable for PDT. Although they have excellent potential for PDT in cancer, the use of their derivatives in clinical settings remains challenging due to limitations in delivery, including poor water solubility and poor tumor selectivity. Therefore, the development of delivery platforms is desirable for the use of PDT as a cancer treatment.

To address these issues, we have developed water-solubilization techniques using supramolecular chemistry strategies, such as host-guest interactions[1] and self-assembly.[2,3] In this study, we will report the approach based on self-assembly using amphiphilic polysaccharides, in which chlorin e6, a clinically used photosensitizer, was introduced. The self-assembly approach can improve not only the stability of chlorin e6 in aqueous media but also its delivery to tumor tissue, mainly via the EPR effect. Owing to their high water content (>99%), self-assembled nanogels facilitate efficient energy transfer to dissolved oxygen, thereby enhancing the generation of reactive oxygen species. We demonstrated their potential as photosensitizers for PDT. The nanogel exhibited an antitumor effect 780-fold higher than that of the clinically available photosensitizer Photofrin. Moreover, Che6P nanogels demonstrated an excellent ability to generate singlet oxygen even in three-dimensional (3D) spheroids, which serve as more complex tumor models. In addition, our system efficiently induced tumor regression comparable to that achieved by Photofrin, without causing harmful side effects. We believe that supramolecular chemistry-based approaches, such as ours, offer unique features with strong potential for application in cancer therapy.

REFERENCES

1. R. Kawasaki, A. Ikeda, On-Off switching of functional guest molecules via exchange of natural product solubilizing agents, *ChemBioChem*, **24**, e202300455, (2023).
2. R. Kawasaki, et. al., Photodynamic therapy using self-assembled nanogels comprising chlorin e6-bearing pullulan, *Journal of Materials Chemistry B*, **9**, 6357-6363. (2021).
3. R. Kawasaki, et. al., Photodynamic therapy using hybrid nanoparticles comprising of upconversion nanoparticles and chlorin e6-bearing pullulan, *Biomaterials Science*, **12**, 5766-5774, (2024).

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Interplay between π-Electronic Circuits and Molecular Aromaticity in Fully Conjugated Asymmetric Multicyclic Macrocycles

Dongho Kim*

Department of Chemistry, Yonsei University, Seoul 03722, Korea

Aromaticity is a central concept in π-conjugated organic molecules, and fully π-conjugated symmetric multicyclic macrocycles have therefore attracted significant attention. In contrast, asymmetric multicyclic systems composed of hetero-sub-macrocycles remain largely unexplored, owing tpotentialheir synthetic advantages, owing tsyntheticо potential challenges. Herein, we describe the synthesis of a series of fully π-conjugated asymmetric multicyclic octaphyrins incorporating bithiophene or benzithiophene subunits, and we examine their redox- and protonation-induced electronic and spin-state modulations associated with aromaticity switching. The neutral species are nonaromatic, but two-electron oxidation induces global aromaticity along the outermost 34-π-electron circuit. Remarkably, protonation generates triplet diradicaloids stabilized by Baird aromaticity. Comprehensive electronic and conformational analyses reveal that these multifaceted changes in aromaticity and spin character originate from cooperative and competing π-electronic interactions between the constituent sub-macrocycles. These findings highlight fundamental design principles for modulating electronic and spin properties in fully conjugated multicyclic macrocycles through controlled interplay of multiple π-electronic circuits.

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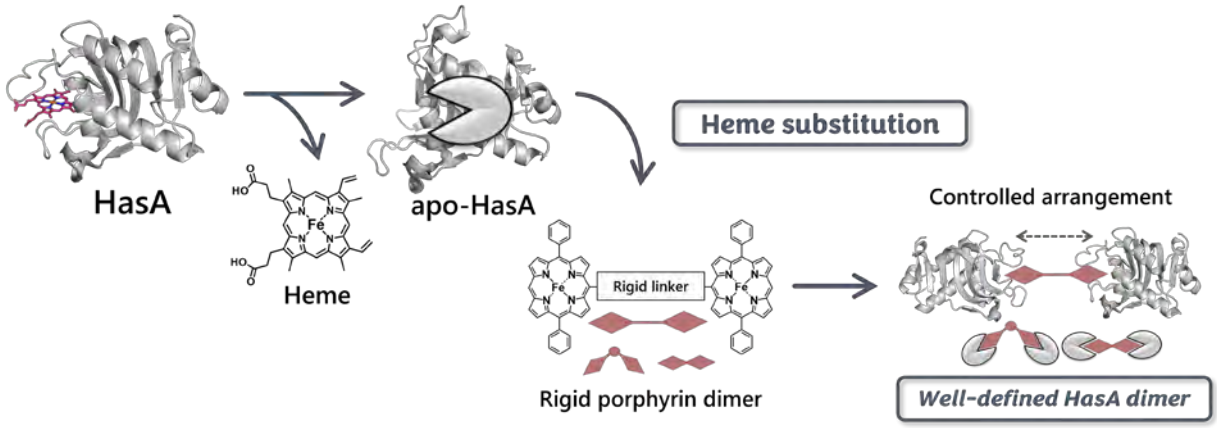
Construction of Artificial Hemoprotein Assemblies by Rational Design of Porphyrin Oligomers

Sukyeong Kim[a], Yuichiro Aiba[a], Hiroshi Sugimoto[b], Osami Shoji[a]

[a]*Graduate School of Science, Nagoya University, Aichi, Japan*
[b]*RIKEN SPring-8 Center Harima Institute, Hyogo, Japan*

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Hemoproteins are among the most versatile metalloproteins and have also been employed as structural building units for artificial protein assemblies. To introduce additional functionalities into hemoproteins for constructing such assemblies, heme substitution with synthetic cofactors is frequently employed [1]. However, the scope of the incorporated synthetic complexes is generally restricted to heme-like molecules, because the heme-binding sites of most hemoproteins are highly optimized for the native heme cofactor.
In contrast, heme acquisition system protein A (HasA), secreted by Gram-negative bacteria, possesses a unique heme-binding site that is highly exposed to solvent. We have found that HasA can capture a variety of rigid metal complexes, including synthetic metalloporphyrins [2,3]. Additionally, we recently succeeded in forming a metal ion-driven HasA dimer by incorporating a porphyrin derivative bearing an additional metal coordination site into HasA [4]. These findings highlight the unique versatility of HasA and enable the construction of well-defined protein assemblies using rationally designed porphyrin oligomers as a structural framework.
In this work, we constructed rigid HasA dimers as an initial step toward well-defined artificial HasA assemblies. Heme substitution with rationally designed rigid porphyrin dimers afforded structurally defined HasA dimers, demonstrating that the porphyrin-linker geometry can precisely control HasA assembly. We further demonstrated that this strategy can be extended to porphyrin trimer frameworks, enabling the formation of HasA trimers that exhibit new functional properties.



REFERENCES

1. K. Oohora and T. Hayashi, *Curr. Opin. Chem. Biol.* **2014**, *19*, 154-161.
2. H. Uehara *et al.*, *Angew. Chem. Int. Ed.*, **2017**, *129*, 15481-15485.
3. Y. Shisaka *et al.*, *ChemBioChem.*, **2022**, *23*, e202200095.
4. H. Inaba *et al.*, *RSC Adv.* **2024**, *14*, 8829-8836.

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Calixpyrrole-Based Ion-Pair Receptors for the Extraction of Lithium and Sodium Salts

Sung Kuk Kim

Gyeongsang National University, Jinju-si, Korea

The selective extraction of lithium and sodium halide salts, whether from solid materials or aqueous solutions, is especially difficult because of their high lattice energies and strong hydration. In this presentation, I will discuss our efforts to tackle this challenge by creating ion-pair receptors that can specifically extract lithium and sodium salts. Our strategy involves designing receptors that combine lithium- or sodium-specific cation-binding units with macrocyclic pyrrolic anion-binding motifs, such as calixpyrroles. Unlike typical receptors that only bind cations or anions, these ion-pair receptors can simultaneously bind both ions. This cooperative binding increases binding strength and enhances selectivity for the desired salts. I will show our findings on the complexation and extraction of lithium and sodium chlorides from both solid and aqueous environments. Additionally, I will explore how solvent effects and the presence of spectator ions impact ion-pair binding and extraction performance.

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Mechanistic Insight into Photogenerated Spin Polarization of Single and Exchange Coupled Spin Systems

Martin L. Kirk[a], **Art van der Est**[b], **David A. Shultz**[c]

[a]*Department of Chemistry and Chemical Biology, The University of New Mexico, Albuquerque, New Mexico 87131-0001*
[b]*Brock University, St. Catharines, Ontario, Canada*
[c]*Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204*

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Abstract: Radical elaborated chromophoric Pt Donor-Acceptor and Donor-*Bridge*-Acceptor ligand-to-ligand charge transfer complexes have been used to control spin-dependent ground and excited state processes that include magnetooptical activity,[1] and ground state electron spin polarization (ESP) [3-5] with quantum information science applications.[6] Although this structural motif has been very successful in generating ground state ESP, the mechanism of ESP generation is still not fully understood.[7] In these radical-elaborated chromophores, photoexcitation with visible light produces an initial exchange-coupled, multi-spin, open-shell excited state that rapidly decays to the ground state via a combination of enhanced intersystem crossing (ISC), exchange-mediated intersystem crossing.[4] Here, we will discuss the role of charge-separated anisotropic exchange to generate zero-field splitting [8] in the chromophore, and how this plays a fundamental role in generating ground state ESP of the pendent radical(s) when the chromophore-radical exchange interaction is large. We will also discuss interesting spin relaxation processes in the ground state of biradical-elaborated chromophores that occur prior to thermalization, which we hypothesize to derive from vibronic spin-orbit coupling between the exchange coupled singlet and triplet states.

REFERENCES

1. Excited State Magnetic Exchange Interactions Enable Large Spin Polarization Effects. Stein, B. W.; Tichnell, C. R.; Chen, J.; Shultz, D. A.; Kirk, M. L., *J. Am. Chem. Soc*. **2018**, *140*, (6), 2221-2228.
2. Chromophore-radical excied state antiferromagnetic exchange controls the sign of photoinduced ground state spin polarization. Kirk, M. L.; Shultz, D. A.; Hewitt, P.; Stasiw, D. E.; Chen, J.; van der Est, A., *Chem. Sci*. **2021**, *12,* (41), 13704-13710.
3. Metal Ion Control of Photoinduced Electron Spin Polarization in Electronic Ground States. Kirk, M. L.; Shultz, D. A.; Chen, J.; Hewitt, P.; Daley, D.; Paudel, S.; van der Est, A., *J. Am. Chem. Soc.* **2021**, *143*, (28), 10519-10523.
4. Bridge Connectivity Effects on Photoinduced Ground-State Electron Spin Polarization. D. A. Shultz, A. R. Marri, A. M. Nogueira, V. K. Mishra M. L. Kirk, and Art van der Est, **2025**. *J. Chem. Phys*. *162*, 8, 084304.
5. Kirk, M. L.; Shultz, D. A.; Hewitt, P.; Marri, A. R.; van der Est, A. Competitive reversed quartet mechanisms for photogenerated ground state electron spin polarization. *Chemical Science* **2023**, *14* (36), 9689-9695.
6. Exploiting chemistry and molecular systems for quantum information science. Wasielewski, M. R.; Forbes, M. D. E.; Frank, N. L.; Kowalski, K.; Scholes, G. D.; Yuen-Zhou, J.; Baldo, M. A.; Freedman, D. E.; Goldsmith, R. H.; Goodson, T.; Kirk, M. L.; McCusker, J. K.; Ogilvie, J. P.; Shultz, D. A.; Stoll, S.; Whaley, K. B., *Nature Reviews Chemistry* **2020**, *4*, (9), 490-504.
7. Kirk, M. L.; Shultz, D. A.; Hewitt, P.; Marri, A. R.; van der Est, A. Competitive reversed quartet mechanisms for photogenerated ground state electron spin polarization. *Chemical Science* **2023**, *14* (36), 9689-9695.
8. Excited Triplet State Zero-Field Splitting in a Ligand-to-Ligand Charge Transfer Complex. J. Mengell, S, Gao, C, Mangione, D, Kersi, S. McGill, D. A. Shultz, and Martin L. Kirk, *J. Chem. Phys*. **2025**, *162*, 164312.

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Synthesis and Biological Application of Artificial Hemoglobin/Myoglobin

Hiroaki Kitagishi

Faculty of Science and Engineering, Department of Molecular Chemistry and Biochemistry, Doshisha University

Hemoglobin and myoglobin are well-known as oxygen-binding proteins in biological systems. Heme cofactors are surrounded by a protein matrix in these proteins, in which the isolation of heme in proteins is essential to achieve reversible oxygen binding in biological systems. To mimic the function of hemoglobin and myoglobin, a water-soluble synthetic porphyrin iron complex (FeTPPS) is encapsulated by per-*O*-methylated b-cyclodextrin (CD) dimer. The 1:1 supramolecular complex of FeTPPS with the CD dimer, named hemoCD, is a water-soluble synthetic hemoglobin and myoglobin model that can reversibly bind molecular oxygen (O_2) in aqueous solution as well as in biological media (in cell cultures and in vivo). Recent studies in our laboratory revealed that hemoCD can bind not only O_2 but also CO, NO, HCH, and H_2S in a reversible manner depending on its iron oxidation state (II/III). Interestingly, the binding tendency of hemoCD is quite similar to that of native hemoglobin and myoglobin. As for application, our hemoCD is superior for use as a chemical antidote against CO, HCN, and H_2S because of its higher binding affinity than native hemes and its rapid urinary clearance from the animal body. The synthesis and application of hemoCD will be overviewed.

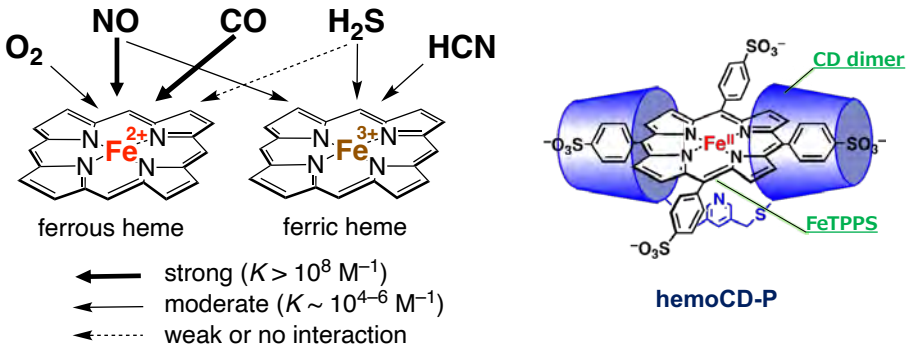


Fig 1. The gas binding tendency to heme (ferric/ferrous) and the structure of hemoCD-P as the first synthetic, water-soluble, and biologically-applicable hemoglobin/myoglobin model.

REFERENCES

(1) H. Kitagishi, K. Kano, *Chem. Commun.* (Feature Article) **2021**, *57*, 148–173.
(2) Q. Mao, H. Kitagishi, et al., *PNAS*, **2023**, 120, e2209924120.
(3) A. Nakagami, H. Kitagishi, et al., *Inorg. Chem.* **2025**, *147*, 13973–13985.
(4) A. Nakagami, H. Kitagishi, et al., *J. Am. Chem. Soc.* **2025**, *147*, 47898–47903.

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Hybrid materials based on metal phthalocyanines and carbon nanotubes: synthesis and sensor properties

Darya Klyamer[a], Victoria Ivanova[a], Pavel Krasnov[b], Tamara Basova[a]

[a]Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia
b International Research Center of Spectroscopy and Quantum Chemistry, Siberian Federal University, Krasnoyarsk, Russia

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Halogenated phthalocyanine-based materials have shown great potential for use in a variety of applications, including organic field-effect transistors, sensors, and biologically related applications [1]. The development of new materials based on MPcHalx remains a key research focus, as it allows for further improvement of the performance characteristics and expansion of the application areas of these materials. Carbon nanotubes (CNTs) serve as excellent platforms for hybrid sensor design due to their large specific surface area and high electrical conductivity [2]. To tailor their sensing performance, CNTs are often functionalized with a variety of compounds, including metal nanoparticles, conjugated polymers, and polyaromatic molecules. Among the latter, metal phthalocyanines (MPc) are of particular interest due to their robust chemical stability, tunable electronic structure, and strong affinity for various gaseous analytes [3].

In this study, we synthesized hybrid materials by both covalently and non-covalently functionalizing both pristine SWCNTs as well as functionalized SWCNTs (SWCNT-COOH, SWCNT-NH_2) with halogenated metal phthalocyanines MPcHalx (x = 0, 4, 8; Hal = F, Cl) derivatives. For comparison, analogous hybrids with unsubstituted MPc were also prepared. The resulting materials were characterized using Fourier-transform infrared (FTIR) and Raman spectroscopy, scanning electron microscopy (SEM) for morphological analysis, and inductively coupled plasma atomic emission spectroscopy (ICP-AES) to quantify the phthalocyanine loading on the nanotube surfaces. Their chemiresistive responses to low concentrations of ammonia and hydrogen sulfide were systematically evaluated at room temperature. To elucidate the origin of observed differences in sensor performance, quantum chemical calculations were performed. By correlating experimental sensing data with theoretical insights into adsorption energetics, this work aims to clarify how phthalocyanine molecular structure and type of nanotubes influence sensitivity. Such understanding will guide the rational design of next-generation chemiresistive sensors with enhanced sensitivity, selectivity, and reliability for real-world applications.

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REFERENCES

1. D. Bonegardt, D. Klyamer, A. Sukhikh, P. Krasnov, P. Popovetskiy, T. Basova. Fluorination vs . Chlorination : Effect on the Sensor Response of Tetrasubstituted Zinc Phthalocyanine Films to Ammonia. Chemosensors 2021, 9, 137.
2. D. Liu, L. Shi, Q. Dai, X. Lin, R. Mehmood, Z. Gu, L. Dai. Functionalization of carbon nanotubes for multifunctional applications. Trends in Chemistry 2024, 6, 186-210.
3. V. Ivanova, D. Klyamer, P. Krasnov, E. N. Kaya, İ. Kulu, S. Tuncel Kostakoglu, M. Durmuş, T. Basova, Sensors Actuators *B* 2023, V. 375, 132843.

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Dual-porphyrin-sensitized photocatalyst for efficient charge separation and solar hydrogen production

Atsushi Kobayashi, Satoshi Odagiri

Department of Marine Resources and Energy, Tokyo University of Marine Science and Technology, 4-5-7 Konan Minato-ku, Tokyo 108-8477, Japan

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Photoinduced charge separation is crucial for converting solar energy to electrical and chemical energy. Since the pioneering work of Grätzel et al. on dye-sensitized solar cells [1], the dye-sensitization technique has been recognized as one of the most effective strategies for harnessing a broad spectral range of solar light in photoelectrochemical devices; this is primarily due to the wide tunability of the light-absorption properties of photosensitizing dyes. We have recently reported on a photoredox cascade catalyst (PRCC) system effective for both hydrogen production and the oxidative synthesis and conversion of organic substrates, and revealed that the key feature enabling its high photocatalytic activity lies in the redox cascade structure formed by two different tris-bipyridyl Ru(II) photosensitizers [2]. To construct the PRCC system based on a nobel-metal-free dye, our recent attention has focused on the redox cascade formation by metalloporphyrin dyes, because the potential of porphyrin-type molecules is demonstrated by their role in natural photosynthesis, where they serve as light-harvesting pigments and electron carriers [3].

In this work, to collaboratively utilize the rapid electron injection at the dye–semiconductor interface and the intermolecular redox reactions between two porphyrin dyes, we synthesized two dual-porphyrin-sensitized Pt-loaded TiO_2 nanoparticle photocatalysts (**ZnP**-Zr-**SnP**@Pt-TiO_2 (**DPSP**) and **SnP**-Zr-**ZnP**@Pt-TiO_2 (**DPSP-r**)) by reversing the loading order of two metalloporphyrin-photosensitizing dyes (**SnP** and **ZnP** = 5,10,15,20-tetrakis(*p*-carboxy phenyl)-porphyrinato-M; M = $Sn^{IV}Cl_2$, Zn^{II}). In a 500 mM *L*-ascorbic acid (AA) sacrificial electron donor aqueous solution, the **DDSP** evolved approximately 10-time larger amount of H_2 and higher turnover number per one porphyrin dye (89.1 μmol, TON = 7314) for 6 h of irradiation of blue light than that of **DDSP-r** (9.1 μmol, TON = 724, see Figure 1), indicating the importance of the loading order of the metalloporphyrin dye for efficient photoinduced charge separation. The barely emissive nature of the **DPSP** and **DPSP-r** and the redox potentials of **ZnP** and **SnP** suggested that the redox cascade structure of the dual-metalloporphyrin **ZnP**-Zr-**SnP** layer plays a key role in photoinduced charge separation for photocatalytic H_2 production. The deital will be discussed.

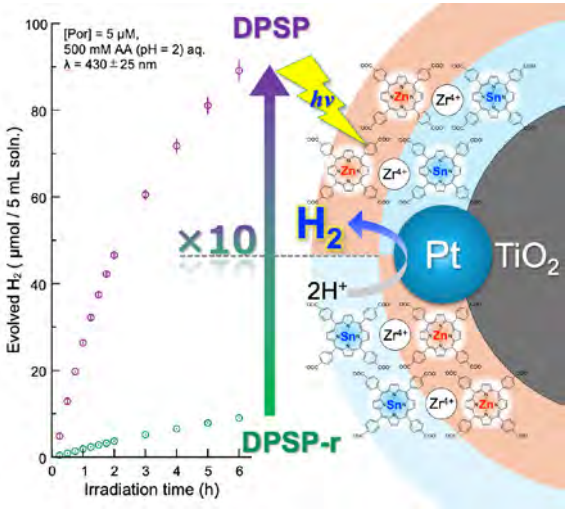


Figure 1. Photocatalytic H_2 production by **DPSP** or **DPSP-r** in 500 mM AA aqueous solution under blue light irradiation.

REFERENCES

1. B. O'Regan, M. Grätzel, *Nature* **1991**, *353*, 737.
2. A. Kobayashi, *ChemSusChem* **2025**, *18*, e202400688.
3. G. D. Scholes, G. R. Fleming, A. Olaya-Castro, R. v. Grondelle, *Nat. Chem.* **2011**, *3*, 763.

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Near Infrared Photoimmunotherapy of Cancer

Hisataka Kobayashi [a,b]

[a] *Molecular Imaging Branch, National Cancer Institute, NIH, Bethesda, MD*
[b] *PhotoImmunotherapy Research Institute, Kansai Medical University, Hirakata, Osaka*

Surgery, radiation, and chemotherapy have been the mainstays of cancer treatment since the advent of modern medicine. Although recent immunotherapies—such as immune-activating cytokines, immune checkpoint inhibitors, engineered T cells, and suppressor-cell depletion—have shown promise, they do not directly destroy cancer cells and rely solely on immune activation; consequently, their efficacy is limited to a subset of patients. To date, no single cancer therapy has successfully achieved both direct cancer cell destruction and simultaneous activation of host anti-tumor immunity. Here, we describe a novel approach using a hydrophilic silicon-phthalocyanine–based photoabsorbing dye, IRDye700DX (IR700), covalently conjugated to monoclonal antibodies (mAbs) that target cancer-specific cell-surface antigens. Upon exposure to near-infrared (NIR) light, these antibody–photoabsorber conjugates (APCs) enable visualization of tumors with low, non-therapeutic NIR light and induce highly selective cancer cell death with therapeutic NIR light—a process termed near-infrared photoimmunotherapy (NIR-PIT).[1,2] When APCs bind to target cancer cells, cytotoxicity is induced within one minute of NIR light exposure, resulting in rapid necrotic and immunogenic cell death. No phototoxicity is observed in adjacent receptor-negative cells in vitro. In vivo, more than 90% cancer cell death has been demonstrated by bioluminescence imaging and ^{18}F-FDG PET following NIR irradiation. With optimized treatment regimens, over 80% of mice achieved tumor-free survival in immunocompetent models, particularly when NIR-PIT was combined with immune-activating strategies such as immune checkpoint inhibitors or immune-suppressive cell-targeted NIR-PIT. IR700 fluorescence also enables image-guided light delivery and post-treatment monitoring, with fluorescence loss indicating adequate therapeutic light exposure. Mechanistically, mAb-IR700–based NIR-PIT is effective only when the conjugate is bound to the cell membrane and induces cytotoxicity via a photo-induced ligand-release reaction, distinct from the reactive oxygen species–dependent mechanisms of conventional photodynamic therapy. Clinically, an FDA-designated fast-track global phase 3 trial is currently ongoing across the US, EU, and Asia. In Japan, the first EGFR-targeted NIR-PIT drug (cetuximab-IR700; Akalux™) and a dedicated NIR light-emitting device (BioBlade™) were approved in September 2020 for recurrent head and neck cancer. Since then, more than 1,100 treatments have been performed in over 700 patients across 180 hospitals. As of summer 2023, pooled clinical data showed an overall response rate of 63.5% and a disease control rate of 84.5%, with outcomes continuing to improve as experience accumulates. [3] In parallel, we have developed next-generation photoabsorbers, the IR702HKT series, designed to further enhance therapeutic efficacy over IR700. In conclusion, mAb-IR700–based NIR-PIT enables highly selective cancer treatment with minimal damage to normal tissues while simultaneously activating robust anti-tumor immunity. This dual mechanism has translated into high complete response rates in clinical practice, establishing NIR-PIT as a transformative cancer therapy now being realized in oncology clinics in Japan.

REFERENCES

1. Mitsunaga M, et al.. Nature Medicine 2011; 17(12): 1685–1691
2. Kobayashi H, Choyke PL. Accounts of Chemical Research 2019;52(8):2332-2339
3. Miyazaki NL, Cancers 2023; 15(21):5117.

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Characteristics of Mononuclear High-Spin Ferric Phthalocyanines: Comparison with Ferric Porphyrins

Nagao Kobayashi,[a] Yusuke Okada,[b] and Hirofusa Shirai[b]

[a]*Department of Chemistry, Faculty of Science, Ochanomizu University, 2-1-1 Otsuka, Bunkyo-ku, Tokyo 112-8610, Japan.*
[b]*Faculty of Textile Science and Technology, Shinshu University, 3-15-1 Tokida, Ueda, Nagano 386-8567, Japan.*

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Iron phthalocyanine (Pc) with eight or four carboxyl groups possesses functions not found in conventional iron porphyrin (P), such as deodorizing and antibacterial properties [1]. Moreover, it is known that its activity is higher when Pc exists as a non-aggregated monomer, such as when it is incorporated into polymers or adsorbed onto fibers [2]. However, these compounds are only soluble in water and tend to aggregate even in aqueous solutions, making it difficult to obtain their properties as individual monomers. Therefore, we decided to esterify them to create a non-aggregating state that is soluble in organic solvents and to investigate their characteristics [3]. These compounds exhibited spectra characteristic of ferric high-spin states in absorption and MCD spectra, and particularly in ESR when dissolved in solvent [4]. However, when aggregated as solid powders, the Mössbauer spectrum showed signals from both ferric high-spin and ferrous intermediate-spin states. Based on the fact that polymer-supported Pc yields only ferric high-spin signals in ESR [3, 4] and exhibits high catalytic activity [2], it was determined that the ferric high-spin species possesses the high deodorizing and antibacterial functions.
Porphyrin (P), tetrabenzoporphyrin (TBP), and Pc are known to exhibit gradual changes in properties due to structural alterations [5]. For ferric high-spin species, it is known that the degree of axial ligand dissociation increases from P to TBP [6]. Thus, while it was expected that this dissociation would increase further for Pc, the fact that axial ligands could not be detected in ferric high-spin Pc prevented verification. On the other hand, analysis of NMR data revealed that for ferric P species, the higher the axial ligand dissociation, the larger the complexation constant value with the base [7]. Therefore, since the complexation constant K_1 between the ferric high-spin Pc species and bases was expected to be very large, we tested its value using various bases. The values were in the order of 10^6 to 10^8, suggesting that even if an axial ligand were present, the ferric high-spin Pc would exhibit extremely high dissociation. To further investigate why axial ligands could not be detected in the ferric high-spin Pc species, we calculated the effective nuclear charge of iron and compared it with those of P and TBP. The values obtained were 2.883, 2.881, and 1.964 for P, TBP, and octacarboxylated Pc, respectively. Since the 1.964 value is less than 2, it was judged reasonable that axial ligands would not attach or be detected.

REFERENCES

[1] (a) Shirai, H.; Maruyama, A.; Takano, J.; Kobayashi, K.; Hojo, N. Makromol. Chem. 1980;**181**: 565. (b) Shirai, H.; Maruyama, A.; Kobayashi, K.; Hojo, N.Makromol. Chem. 1980; **181**: 575.
[2] (a) Shirai, H.; Maruyama, A.; Kobayashi, K.; Hojo, N. J. Polym. Sci. Polym. Lett. Ed. 1979; **17**: 661. (b) Shirai, H.; Higaki, S.; Hanabusa, K.; Hojo, N. J. Polym. Sci. Polym. Lett. Ed. 1983; **21**: 157. (c) Shirai, H.; Higaki, S.; Hanabusa, K.; Kondo, Y.; Hojo, N. J. Polym. Sci. Polym. Chem. Ed. 1984; **22**: 1309.
[3] (a) Kobayashi, N.; Koshiyama, M.; Funayama, K.; Osa, T.; Shirai, H.; Hanabusa, K.. J. Chem. Soc, Chem. Commun. 1983; 913. (b) Okada, Y.; Kobayashi, N. J. Inorg. Biochem. 2025; **262**: 112737.
[4] Kobayashi, N.; Shirai, H.; Hojo, N. J. Chem. Soc., Dalton Trans.1984; 2107.
[5] Mack, J.; Stillman, M.J. in "The Porphyrin Handbook" eds. Kadish, K. M.; Smith, K. M.; Guilard, R. Academic Press, New York, 2003; **16**: 43.
[6] Kobayashi, N.; Koshiyama, M.; Osa, T. Inorg. Chem. 1985; **24**: 2502.
[7] Walker, F.A.; Lo, M.W.; Ree, M.T. J. Am. Chem. Soc. 1976; **98**: 5552.

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Biocompatible Polymer-Conjugated Hemoglobins: Artificial O_2 Carriers as Red Blood Cell Substitutes

Teruyuki Komatsu

Deprtment of Applied Chemistry, Faculty of Science and Engineering, Chuo University, 1-13-27 Kasuga, Bunkyo-ku, Tokyo 112-8551, Japan

ORALS

Blood transfusion products are entirely dependent on donations from volunteers. Recently, declining birthrates and aging populations have led to a global decrease in donor availability, posing a critical challenge to healthcare systems. The COVID-19 pandemic in 2020 further exacerbated this issue by causing severe blood shortages that disrupted routine medical services. Consequently, there is an urgent global need to develop artificial blood products, particularly red blood cell (RBC) substitutes. Over the past several decades, numerous hemoglobin (Hb)-based O_2 carriers (HBOCs) have been developed and evaluated. Among these, polyethylene glycol (PEG)-conjugated Hbs (PEG-Hbs) have been extensively studied as promising artificial O_2 carriers. However, several researchers have reported the formation of anti-PEG antibodies, which have been detected in approximately 43% of healthy individuals [1].

As an alternative to PEG, poly(2-ethyl-2-oxazoline) (POx) have attracted considerable attention due to its properties, such as nonionicity, chain flexibility, and high solubility, comparable to those of PEG, while offering superior immunological stealth capability [2]. In this study, we characterized POx-conjugated Hbs (POx-Hbs) from both physicochemical and physiological perspectives, evaluating its potential as a next-generation artificial O_2 carrier. POx-Hb was synthesized by coupling surface lysine residues on Hb with a sulfhydryl-terminated POx derivative [3]. The resulting POx-Hb solution exhibited lower colloid osmotic pressure than its PEG-Hb counterpart. The O_2 affinity of POx-Hb, as indicated by its P_{50} value (the O_2 partial pressure at which Hb is 50% saturated), was measured at 9 Torr. Furthermore, POx-Hb^L, synthesized under an N_2 atmosphere, displayed reduced O_2 affinity (P_{50} = 57 Torr) [4]. By blending POx-Hb with POx-Hb^L, the P_{50} of the final formulation could be finely tuned to meet specific physiological requirements.

The POx-Hb formulation demonstrated excellent hemocompatibility, showing no adverse effects on platelet, granulocyte, or monocyte function. In vivo pharmacokinetic studies in rats revealed that POx-Hb had a circulation half-life 14 times longer than that of unmodified Hb. Therapeutic efficacy was confirmed in a rat model of 50% hemorrhagic shock, where infusion of the POx-Hb solution resulted in significant improvements in circulatory parameters [3]. Serum biochemical analyses and histopathological examinations indicated no signs of acute toxicity or organ-specific abnormalities. These results highlight POx-Hb as a highly promising RBC substitute with strong potential for application as a therapeutic O_2 carrier in transfusion medicine. The similar biocompatible polymer-conjugated Hb formulation will also be presented.

REFERENCES

1. B.-M. Chen, T.-L. Cheng, S. R. Roffler, *ACS Nano* **2021**, *15*, 14022.
2. M. Glassner, M. Vergaelen, R. Hoogenboom, *Polym. Int.* **2018**, *67*, 32.
3. W. Okamoto, Y. Hiwatashi, T. Kobayashi, Y. Morita, H. Onozawa, M. Iwazaki, M. Kohno, H. Tomiyasu, R. Tochinai, R. Georgieva, H. Bäumler, T. Komatsu, *ACS Appl. Bio Mater.* **2023**, *6*, 3330.
4. R. Wakabayashi, K. Ishii, T. Yamada, T. Komatsu, *Macromol. Chem. Phys.* **2025**, *226*, 2400183.

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Magnetic and optical properties of anionic metallomacrocycles

Konarev D.V.,*[a] Faraonov M.A.,[a] Romanenko N.R.,[a] Nazarov D.I.,[a] Otsuka A.[b]

[a]*Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS Chernogolovka, 142432 Russia*; E-mail: konarev3@yandex.ru,
[b]*Division of Chemistry, Graduate School of Science, Kyoto University, Sakyo-ku, Kyoto 606-8502, Japan.*

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Metallomacrocycles are widely used for the preparation of functional organic materials. They can contain paramagnetic metal ions and radical anion macrocycles. As a result, magnetic assemblies based on them can show magnetic transitions associated with metal-to-macrocycle charge transfer or transitions to a high-spin state. Different metal fragments, including paramagnetic ones, can coordinate to tin(II) or indium(III) macrocycles having diamagnetic (2-), (4-) and paramagnetic (•3-) states [1]. Reduction of tetraphenylporphyrins (TPP) and hemihexaphyrazines (Hhp) yields $\{Crypt(Cs^+)\}\{Ni^I(TPP^{2-})\}^-$ and $\{Crypt(Cs^+)\}_2\{Ni^{II}_2Ni^IO(Hhp^{5-})\}^{2-}$ with paramagnetic nickel(I) (S = 1/2). The increase in magnetic moment is observed in both compounds due to electron transfer or the transition of Hhp^{5-} to the triplet excited state. On the contrary, magnetic exchange between paramagnetic Cu^{II}_3O (S =1/2) and $Hhp^{\bullet 6-}$ (S=1/2) spicies is observed in $\{Crypt(Cs^+)\}_2\{Cu^{II}_3O(Hhp^{\bullet 6-})\}^{2-}$. $\{Crypt(K^+)\}_2\{Co^{II}Co^I_2O(Hhp^{\bullet 4-})\}^{2-}$ contains paramagnetic Co^{II} ion and $Hhp^{\bullet 4-}$. The increase in magnetic moment is attributed to electron transfer from Co^I to $Hhp^{\bullet 4-}$ followed by the formation of $\{(Co^ICo^{II}_2O)^{3+}(Hhp^{5-})\}^{2-}$ [2]. Di- and tri-nuclear assemblies of metallomacrocycles can also show promising magnetic properties. Depending on charge transfer from a bridged ligand to a metal ion (Fe^{III} or Mn^{III}), the {(MTPP)$_2$(thioindigo)} assemblies can show strong antiferromagnetic coupling of spins, transfer to a high-spin (S = 5) state with a parallel arrangement of three spins, or the M-thioindigo coupling can be suppressed by the decrease in the angle between the thioindigo and the porphyrin plane [3]. Tri-nuclear complexes are also obtained when low-spin $\{Mn^{II}(CN)_2Pc\}^{2-}$ (S = 1/2) bridge mediates magnetic coupling between high-spin $Mn^{II}(acac)_2$ (S = 5/2) or Cp_3Gd^{III} (S = 7/2) in $\{Crypt(K^+)\}_2\{Mn^{II}(CN)_2Pc[Mn^{II}(acac)_2$ (or $Cp_3Gd^{III})]_2\}$. In the first case, a high-spin assembly with S = 9/2 spin state is obtained. Manganese(II) tetraphenylporphyrin also forms di- and tri-nuclear assemblies. Diamagnetic violanthrone^{2-} dianion and low-spin $\{Mn^{II}(triazole)_2Pc\}^{2-}$ (S = 1/2) dianions as bridges provide weak antiferromagnetic coupling of spins or transfer a compound to a high (S = 9/2) spin state [4]. External coordination of two paramagnetic metal centers (M= Co^{II}, Fe^{II}, Dy^{III}) to iron(II) octaethyltetrapyrazinoporphyrazine yields tri-nuclear $(TBA^+)_2\{Fe^{II}I_2$ $(OEtTPrzPz^{2-})[MI_{2(3)}]_2\}$ assemblies with antiferromagnetic coupling of spins. This work was supported by the Russian Science Foundation (№ 24-13-00060).

REFERENCES

1. M. A. Faraonov, A.V. Kuzmin, S. S. Khasanov, S. I. Troyanov, E. I. Yudanova, A. Otsuka, H. Yamochi, H. Kitagava, D. V. Konarev, *CrystEngComm*, 2023, **25**, 4620.
2. D. I. Nazarov, A.V. Kuzmin, M.K. Islyaikin, E.N. Ivanov, A.F. Shestakov, M.A. Faraonov, S.S. Khasanov, A. Otsuka, H. Yamochi, H. Kitagawa, D.V. Konarev, *New J. Chem.*, 2025, **49**, 1631.
3. D. I. Nazarov, M.A. Faraonov, S.M. Nations, L.G. Gutsev, I.A. Yakushev, A.V. Kuzmin, S.S. Khasanov, A. Otsuka, H. Yamochi, H. Kitagawa, D.V. Konarev, *Inorg. Chem*., 2024, **63**, 22677.
4. D. I. Nazarov, M. A. Faraonov, A.V. Kuzmin, S.S. Khasanov, A. Otsuka, H. Yamochi, H. Kitagawa, D.V. Konarev, *Dyes and Pigm.*, 2024, **223**, 111926.

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Molecular Assembly for Small Molecule Conversions

Mio Kondo[a]

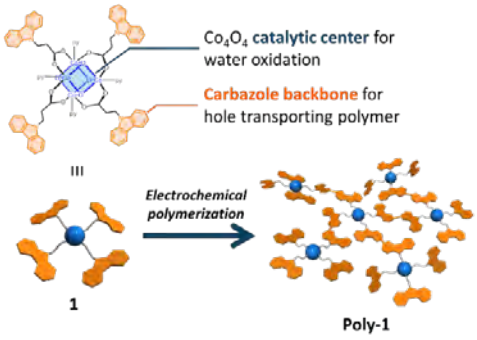
[a] *Department of Chemistry, School of Science, Institute of Science Tokyo*

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Development of catalysts for small-molecule conversion reactions has drawn tremendous attention recently as one of solutions to energy and environmental problems. In particular, the catalysts that can produce sustainable fuels and chemicals from abundant sources are highly desirable. In nature, small molecular conversions are efficiently promoted by catalytic systems in which a catalytic center and surrounding reaction field such as charge transporting sites and accumulation sites for substrates are synergistically integrated. Therefore, the construction of reaction field suitable for the catalysis is expected to be essential to drive small molecule conversion efficiently in artificial catalytic systems. In this study, we aimed to construct novel catalytic systems for small molecule conversion by controlling reaction fields surrounding catalytic centers via molecular assembly.

First, we have succeeded in the development of efficient catalytic system for water oxidation. Water oxidation is a key reaction in natural and artificial photosynthesis. In nature, the reaction is efficiently catalyzed by a metal-complex-based catalyst surrounded by hole-transporting amino acid residues. However, in artificial systems, there is no example of the water oxidation system which has a catalytic center surrounded by hole transporters. Here, we present a facile strategy to integrate catalytic centers and hole transporters into one system. Electrochemical polymerization of a metal-complex-based precursor afforded the polymer-based material (**Poly-1**). **Poly-1** exhibits excellent hole-transporting ability and catalyzes water oxidation with high performance. It was also revealed that the catalytic activity was almost suppressed in the absence of the hole-transporting moieties[1]. We also confirmed the versatility of our strategy for constructing efficient catalytic systems for water oxidation[2]. The study provides a novel strategy for constructing efficient molecule-based systems for water oxidation.

Second, we have succeeded in developing catalytic systems for CO_2 reduction. The development of catalysts for CO_2 reduction is of great significance for constructing a sustainable energy cycle. Here, we report that the control over reaction fields affords efficient catalytic systems for CO_2 reduction. In this study, we have controlled the reaction fields by using the concept of framework catalyst. The introduction of the concept of framework catalyst provided a novel catalyst which possesses (a) catalytic center, (b) capturing sites for CO_2, and (c) accumulation sites for CO_2, as a result, CO_2 reduction reaction selectively promoted even in aqueous solutions[3]. We also revealed that the framework catalyst can function as highly efficient catalyst for photochemical CO_2 reduction[4].



REFERENCES

1. H. Iwami, M. Okamura, M. Kondo, S. Masaoka, *Angew. Chem. Int. Ed*. **2021**, *60*, 5965.
2. T. Matsuzaki, K. Kosugi, H. Iwami, T. Kambe, Y. Harada, D. Asakura, T. Uematsu, S. Kuwabata, Y. Saga, M. Kondo, S. Masaoka, *Nat. Commun.*, **2025**, *16*, 2145.
3. M. Tasaki, Y. Okabe, H. Iwami, C. Akatsuka, K. Kosugi, K. Negita, S. Kusaka, R. Matsuda, M. Kondo, S. Masaoka, *Small*, **2021**, 2006150.
4. K. Kosugi, C. Akatsuka, H. Iwami, M. Kondo, S. Masaoka, *J. Am. Chem. Soc*., **2023**, *145*, 10451.

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Construction of Highly Efficient Molecular Catalytic Systems for CO_2 Reduction by Controlling Reaction Fields

Kento Kosugi[a]

[a]*School of Science, Institute of Science Tokyo*

The development of artificial molecular catalysts for CO_2 reduction is important to solve energy and environmental problems. So far, we have developed highly efficient catalysts for that purpose based on the effects of the reaction field.[1-5] Here, we report the simple procedures that dramatically enhance electrochemical CO_2 reduction activity by metal porphyrin complexes focusing on the effect of the reaction medium.[1,2]

We began by reinvestigating CO_2 reduction by a commercially available catalyst, iron(III) tetraphenylporphyrin chloride (**FeTPP-Cl**), in DMF. DMF is a conventional solvent for iron porphyrin systems, as it can dissolve both the complex and CO_2 at high concentration. **FeTPP-Cl** indeed exhibited a large irreversible current under CO_2, corresponding to the electrocatalytic reduction of CO_2 (Figure 1, red line). Unexpectedly, the intensity of the irreversible current increased when acetonitrile (MeCN) was added (Figure 1, dashed lines). Furthermore, **FeTPP-ClO$_4$**, a perchlorate salt of **FeTPP** that is well soluble in various solvent, exhibited the largest irreversible current in pure MeCN (Figure 1, blue line). To quantify the catalytic product, controlled potential electrolysis experiment of **FeTPP-ClO$_4$** was then performed in MeCN with TFE under CO_2 at –2.35 V vs. Fc/Fc^+. The total amount of charge passed over a period of 60 min was 75.9 C, and CO was formed with a Faradaic efficiency of 97.3%. Subsequently, turnover frequency (TOF) for CO production was evaluated. Surprisingly, TOF reached 7.30×10^6 s^{-1}, which is the highest among those of current best-in-class molecular catalysts. These results clearly demonstrate that the electrocatalytic activity of **FeTPP** for CO_2 reduction is significantly enhanced in MeCN.

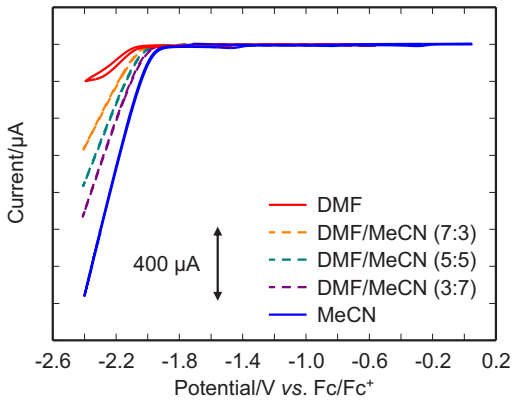


Figure 1. Cyclic voltammograms of **FeTPP** in TBAP/solvent under CO_2 with 1.0 M TFE (scan rate: 100 mV s^{-1}).

The effect of reaction medium on the catalytic activity was also observed for other metal porphyrin complex.[2] In MeCN, a copper porphyrin complex bearing strong electron-withdrawing substituents, copper(II) tetrakis(pentafluorophenyl)porphyrin, exhibited a TOF of 1.46×10^6 s^{-1} at an overpotential of 0.85 V. The details of the reaction medium on the catalytic mechanisms will be discussed in the presentation.

REFERENCES

1. Kento Kosugi, Mio Kondo, and Shigeyuki Masaoka, *Angew. Chem. Int. Ed.*, **2021**, *60*, 22070-22074.
2. Kento Kosugi, Hina Kashima, Mio Kondo, and Shigeyuki Masaoka, *Chem. Commun.*, **2022**, *58*, 2975-2978.
3. Kento Kosugi, Maho Imai, Mio Kondo, and Shigeyuki Masaoka, *Chem. Lett*, **2022**, *51*, 224-226.
4. Kento Kosugi, Chiraru Akatsuka, Hikaru Iwami, Mio Kondo, and Shigeyuki Masaoka, *J. Am. Chem. Soc.*, **2023**, *145*,19, 10451–10457.
5. Maho Imai, Kento Kosugi, Yutaka Saga, Mio Kondo, and Shigeyuki Masaoka, *Chem. Commun.*, **2023**, *59*, 10741-10744.

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Far-red light-harvesting Chl *a*/*b* binding protein complex allows uphill energy transfer for photosynthesis in an Antarctic alga

Makiko Kosugi[a,b], Keisuke Saito[c,d], Yusuke Yoneda[b,e], Masato Kawasaki[b,f], Yutaka Shibata[g], Kojiro Hara[h], Shinichi Takaichi[i], Toshio Moriya[f], Naruhiko Adachi[f,j], Yasuhiro Kamei[a,b], Yasuhiro Kashino[k], Sakae Kudoh[b,l], Hiroyuki Koike[m], Toshiya Senda[b,f], Hikaru Kuramochi[b,e,n], Hiroshi Ishikita[c,d], Jun Minagawa[a,b]

[a]*National Institute for Basic Biology*, [b]*Graduate Institute for Advanced Studies, SOKENDAI*, [c]*Department of Applied Chemistry, The University of Tokyo*, [d]*Research Center for Advanced Science and Technology, The University of Tokyo*, [e]*Reserch Center of Integrative Molecular Systems, Institute for Molecular Science*, [f]*High Energy Accelerator Research Organization (KEK)*, [g]*Graduate School of Science, Tohoku University*, [h]*Akita Prefectural University*, [i]*Tokyo University of Agriculture*, [j]*Life Science Center for Survival Dynamics*, *Tsukuba University*, [k]*Graduate School of Science*, *University of Hyogo*, [l]*National Institute of Polar Research*, [m]*Chuo University*, [n]*Graduate School of Engineering Science, The University of Osaka*

Prasiola crispa, an aerial green alga, forms layered colonies under the severe terrestrial conditions of Antarctica. Since only far-red light is available at a lower layer of the colony, *P. crispa* has evolved a molecular system for photosystem II (PSII) excitation using far-red light with uphill energy transfer [1]. Recently, we identified a light-harvesting chlorophyll (Chl)-binding protein complex in *P. crispa* (Pc-frLHC) that excites PSII with far-red light and revealed that it has a ring-shaped structure with undecameric 11-fold symmetry at 3.13Å resolution [2]. Each LHC-like subunit has four transmembrane helices and binds 11 Chls and two carotenoids (loroxanthin and violaxanthin). Combining spectroscopic analyses with a quantum mechanical/molecular mechanical approach, we identified the far-red–absorbing Chl(s) (far-red Chls). The Chl 603-609 dimer exhibits the strongest excitonic coupling. This dimer also exhibits the largest excitation-induced permanent dipole moment along the axis connecting the two Chls, reflecting the most pronounced charge-transfer character [3].

Transient absorption anisotropy resolved a characteristic hopping time between the far-red Chl trimers of ~11.5 ps. Spectral dynamics and anisotropy further revealed the existence of a higher-lying excitonic state near ~670 nm within the far-red Chls. Thermal access to this level enables repeated cycling that facilitates the uphill transfer toward Chl despite a sizable energy gap of ~580 cm^{-1}[4]. These findings clarify how Pc-frLHC exploits the excitonic coupling and the ring-mediated transport to harvest far-red light energy for PSII excitation.

REFERENCES

1. Kosugi, M. et al., Red-shifted chlorophyll *a* bands allow uphill energy transfer to photosystem II reaction centers in an aerial green alga, Prasiola crispa, harvested in Antarctica. *BBA* 1861(2):148139, 2020.
2. Kosugi, M. et al., Uphill energy transfer mechanism for photosynthesis in an Antarctic alga. *Nat Commun*. 14(1):730, 2023.
3. Saito, K. et al., Identification and design principles of far-red-absorbing chlorophyll in the light-harvesting complex. *J Biol Chem*. 108518, 2025.
4. Yoneda, Y. et al., Upper-state-assisted uphill energy transfer in a far- red light-harvesting antenna from an Antarctic alga. *ChemRxiv*. 2025; doi:10.26434/chemrxiv-2025-d3vc7

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Photocatalytic formation of hydrogen (H_2) and hydrogen peroxide (H_2O_2) catalyzed by nonplanar porphyrins

Hiroaki Kotani, Takahiko Kojima

Department of Chemistry, Faculty of Pure and Applied Sciences, University of Tsukuba

Development of light-induced production of hydrogen (H_2) evolution and hydrogen peroxide (H_2O_2) is indispensable for constructing a sustainable society on the basis of the effective utilization of solar energy because H_2 and H_2O_2 are able to be converted to electrical energy using fuel-cell technology. For achieving the goal, we have focused on saddle-diprotonated dodecaphenylporphyrin (H_4DPP^{2+}) derivatives as a near-infrared (NIR)-light-responsive photosensitizer and as a selective O_2-reduction catalyst.[1] Here, we report NIR light-driven H_2 evolution catalyzed by a combination of a diprotonated saddle-distorted porphyrin as a photosensitizer and platinum nanoparticles as H_2-evolving catalysts.[2,3] Under the optimized conditions, a turnover number of NIR light-driven H_2 evolution reached 1600 at 1 h with the 80% yield of H_2 based on a sacrificial electron donor. The quantum yield of H_2 evolution at 750 nm was determined to be 36%, which is the highest value among photocatalytic H_2-evolution systems based on NIR irradiation reported so far (Figure 1).[3] The H_2-evolution mechanism was elucidated on the basis of femto-second and nano-second laser flash photolysis.

On the other hand, we designed an organic-inorganic hybrid photocatalyst for the production of H_2O_2 by using water as an electron source. The hybrid photocatalyst was prepared by immobilizing a H_4DPP^{2+} derivative as an O_2-reduction catalyst on the surface of TiO_2, which was employed for a water-oxidation catalyst. When the H_4DPP^{2+}-TiO_2 hybrid photocatalyst dispersed in pure water was irradiated at 365 nm using an LED lamp under air, formation of H_2O_2 was confirmed by iodometry of the supernatant. The amount of H_2O_2 was determined to be 0.3 mM under photoirradiation for 60 seconds and the external quantum yield at 365 nm reached to 28%, which is the highest value among semiconductor photocatalysts reported so far for H_2O_2 production.[4]

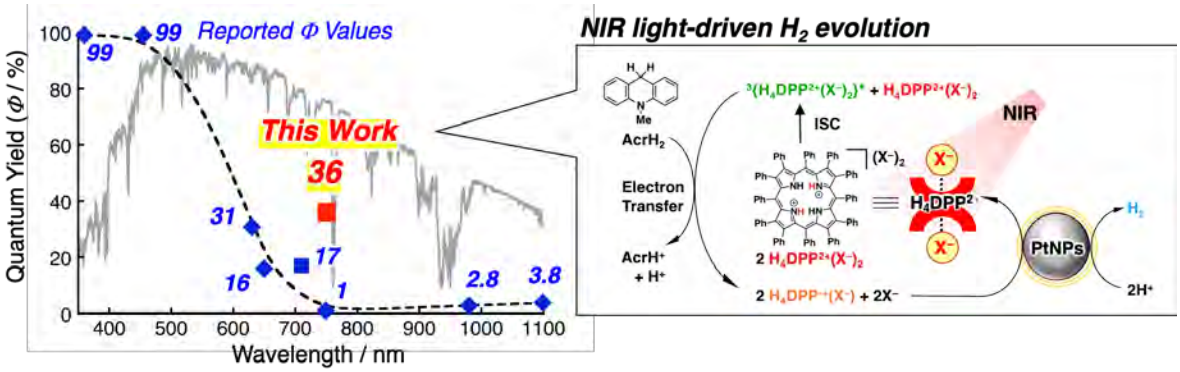


Figure 1. Schematic illustration of NIR-light-driven H_2 evolution catalyzed by $H_4DPP^{2+}(X^-)_2$ [3]

REFERENCES

1. T. Ishizuka, N. Grover, C. J. Kingsbury, H. Kotani, M. O. Senge, T. Kojima, *Chem. Soc. Rev.* **2022**, *51*, 7560.
2. H. Kotani, T. Miyazaki, E. Aoki, H. Sakai, T. Hasobe, T. Kojima, *ACS Appl. Energy Mater.* **2020**, *3*, 3193.
3. H. Kotani *et al.*, *ChemPhotoChem* **2025**, *9*, e202500009.
4. H. Kotani *et al.*, submitted for publication.

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B_{12} - from Vitamin to Antivitamin B_{12}

Bernhard Kräutler

Institute of Organic Chemistry, University of Innsbruck, Innsbruck, Austria bernhard.kraeutler@uibk.ac.at

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The natural vitamin B_{12} derivatives are fascinatingly complex cobalt corrins [1] The preeminent use of cobalt in the B_{12}-cofactors [1-3] has stimulated the quest for understanding the specific biological selection of cobalt, inducing a fundamental interest in finding ways of replacing cobalt by other transition metals. [4-8] The seemingly attractive direct substitution of cobalt by rhodium is a chemically inaccessible path from the natural cobalt-corrins to their rhodium analogues. Thus, successful synthetic roads to rhodium analogues of the natural cobalt-corrinoids start with metal-free corrinoids, [1,4,6] most rationally with crystalline metal-free hydrogenobyric acid.[9]

The so far studied Rh-corrins are remarkably isostructural to their natural Co-corrin analogues,[5,10-12] but lack their biologically crucial fine-tuned reactivity. [5,6,8-12] In consequence, the rhodium analogues of the B_{12}-cofactors have features of very effective antivitamins B_{12},[8,12,13] as well as of inhibitors of specific B_{12}-enzymes, of B_{12}-dependent photoregulation of gene expression and of growth of B_{12}-dependent microorganisms. They are particularly promising candidates for chemical and structural biological, [13] and biomedical [12,14] applications.

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REFERENCES

[1] A. Eschenmoser, Angew. Chem. Int. Ed., 27 (1988) 5-39.
[2] J.M. Pratt, Inorganic Chemistry of Vitamin B_{12}, Academic Press, New York, 1972.
[3] B. Kräutler, B. Puffer, Handbook of Porphyrin Science, Vol. 25 (Eds.: K.M. Kadish, Smith, K.M., Guilard, R.), World Scientific, 2012, pp. 131-263.
[4] V.B. Koppenhagen, Metal-Free Corrinoids and Metal Insertion, in: D. Dolphin (Ed.) B_{12}, John Wiley & Sons, 1982, pp. 105-150.
[5] F.J. Widner, A.D. Lawrence, E. Deery, D. Heldt, S. Frank, K. Gruber, K. Wurst, M.J. Warren, B. Kräutler, Angew. Chem. Int. Ed. 55 (2016) 11281-11286.
[6] B. Kräutler, Chem. Eur. J., 26 (2020) 15438-15445.
[7] F. Zelder, R. Alberto, Handbook of Porphyrin Science Vol. 25 (Eds.: K.M. Kadish, Smith, K.M., Guilard, R.), World Scientific, 2012, pp. 84-132
[8] B. Kräutler, in Vitamins and Hormones, Vol. 119 (Ed.: G. Litwack), Academic Press, Cambridge, Mass., 2022, pp. 221-240.
[9] C. Kieninger, E. Deery, A.D. Lawrence, M. Podewitz, K. Wurst, E. Nemoto-Smith, F.J. Widner, J.A. Baker, S. Jockusch, C.R. Kreutz, K.R. Liedl, K. Gruber, M.J. Warren, B. Kräutler, Angew. Chem. Int. Ed. 58 (2019) 10756-10760.
[10] F.J. Widner, C. Kieninger, K. Wurst, E. Deery, M.J. Warren, B. Kräutler, Synthesis 53 (2021) 332–337.
[11] M. Wiedemair, C. Kieninger, K. Wurst, M. Podewitz, E. Deery, M. D. Paxhia, M. J. Warren, B. Kräutler, Helv Chim Acta 2023, 106, e202200158.
[12] F. J. Widner, K. Wurst, M. Ruetz, C. Kieninger, C. Kreutz, M. D. Paxhia, E. Deery, M. J. Warren and B. Kräutler, *ChemistryEurope*, 2025, **3**, e202500157.
[13] M. Ruetz, R. Mascarenhas, F. Widner, C. Kieninger, M. Koutmos, B. Kräutler and R. Banerjee, *Biochemistry*, 2024, **63** 1955–1962.
[14] F. Zelder, M. Sonnay, L. Prieto, ChemBioChem, 16 (2015) 1264-1278.

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Comparing FeN_4 motifs with either pyridinic or pyrrolic coordination for the activation of oxygen

Kosovare Zullufi[a], Anusree Ghosh[b], Nicole Segura-Salas[a], Lingmei Ni[a], Herbert Plenio[b], Ulrike I. Kramm[a]

[a] *Technical University of Darmstadt, Department of Chemistry, Eduard Zintl Institute of Inorganic and Physical Chemistry, Catalysts and Electrocatalysts, Otto-Berndt-Str. 3, 64287 Darmstadt, Germany*
[b] *Technical University of Darmstadt, Department of Chemistry, Eduard Zintl Institute of Inorganic and Physical Chemistry, Inorganic and Organometallic Chemistry, Peter-Grünberg-Str. 12, 64287 Darmstadt, Germany*

FeN_4 macrocycles immobilized on carbon are applicable to various electrocatalytic reactions. They also serve as model systems for so-called iron-nitrogen-carbon (FeNC) catalysts, where it is believed that the catalysis-relevant moieties also comprise square-planar N_4 coordination but embedded into a graphene layer rather than molecular surroundings as in the case of the macrocycles. It is suggested that in these graphene sheets, the coordinating nitrogen atoms are either of pyridinic or pyrrolic nature. However, FeNC catalysts are highly amorphous and composed of several structural motifs that may even differ among preparation approaches. As such, the relationship between several aspects and oxygen reduction reaction (ORR) catalysis remains unclear. However, their high potential for application in proton exchange membrane and alkaline fuel cells motivates a more fundamental understanding.[1]

Based on this, in this work, we compare the cyclic voltammetry and oxygen reduction reaction catalysis of iron phthalocyanine vs. iron bipyridine, both immobilized on carbon. The performance is evaluated under different iron utilization levels to identify the optimal conditions. Mössbauer measurements are performed to identify hyperfine interaction parameters, which are then compared across different types of FeNC materials.[2]

It is shown that the redox behaviour changes significantly with iron coordination and that this affects the material's activity and selectivity.

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REFERENCES

1. Kramm UI, Elbaz L. Modifying Fe-N Interaction to Boost Catalytic Performance, *Nature Catalysis*, 6 (2023), 1111.
2. Ni L, Gallenkamp C, Paul S, Kübler M, Theis P, Chabbra S, Hofmann K, Bill E, Schnegg A, Albert B, Krewald V, Kramm UI. Active Site Identification in FeNC Catalysts and Their Assignment to the Oxygen Reduction Reaction Pathway by In Situ ^{57}Fe Mössbauer Spectroscopy, *Advanced Energy and Sustainability Research*, 2 (2021) 2000064.

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Expanding the porphyrinoid toolbox: recent progress in the carbene transfer catalyzed with tetrapyrrolic complexes

Andrey P. Kroitor[a,c], **Alexander A. Dmitrienko** [a,b], **Cenna Toullec** [c], **Alexander G. Martynov**[a], **Yulia G. Gorbunova**[a,b], **Alexander B. Sorokin**[c]

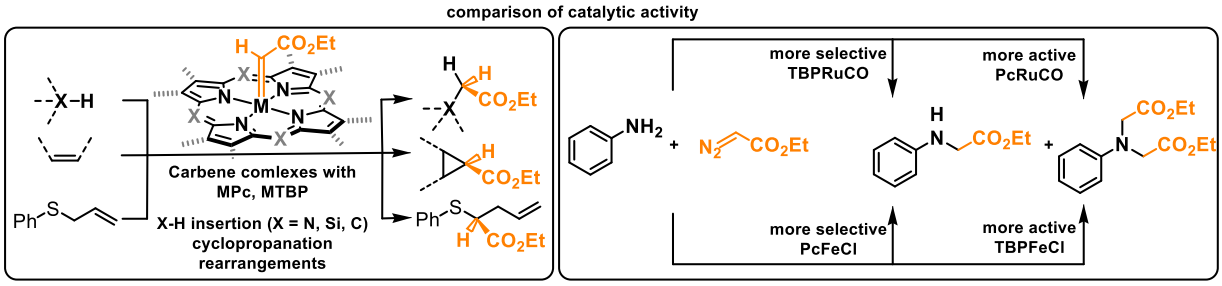
[a] *Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, 31-4 Leninsky Prospect, 119071 Moscow, Russia*
[b] *Lomonosov Moscow State University, Department of Chemistry, Leninskie Gory, 1-3, Moscow 119991, Russia*
[c] *Institut de Recherches sur la Catalyse et l'Environnement de Lyon IRCELYON, UMR 5256, CNRS – Université Lyon 1, 2 av. A. Einstein, 69626 Villeurbanne, France*
[d] *Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, 31 Lenisky Prospect, 119991 Moscow, Russia*

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Carbene transfer reactions represent a powerful and atom-economical tool for the construction of various C–X bonds. In particular, porphyrin complexes have emerged as highly efficient catalysts for carbene insertion into X–H (X = N, S, Si, C) bonds and for diastereo- and enantioselective cyclopropanation. Despite the structural diversity of tetrapyrrolic compounds, the implementation of other porphyrinoid complexes in carbene transfer reactions has remained sporadic and scarce, although we have already shown that phthalocyanine complexes reveal superior activity in cyclopropanation and insertion of carbene to N-H bond [1-3].

Herein we report our recent results of comparative investigation of Cu(II), Co(II), Mn(III), Fe(III) and Ru(II) phthalocyanines and tetrabenzoporphyrins complexes as catalysts for carbene transfer from ethyl diazoacetate to different substrates (e.g., styrene, aniline, triethylsilane, xanthene, phenylallyl sulfide). The highest activity was observed for the ruthenium and iron complexes. The selectivity and activity of the catalyst for carbene insertion into N-H bonds are influenced by both the metal center and the ligand structure. These results demonstrate that selective routes to secondary and tertiary amines can be achieved not only by modifying substituents on a macrocyclic framework but also by employing novel, previously unexplored tetrapyrrolic scaffolds.

Overall, these findings encourage further catalyst development to broaden their applicability to other reaction types and to attain high selectivity in more demanding transformations.



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REFERENCES

1. Cailler LP et al. *Dalton Trans.* 2021; **50**: 2023-2031.
2. Kroitor AP et al. *Org. Biomol. Chem.* 2023; **21**: 69-74.
3. Kroitor AP et al. *ACS Catal.* 2025; **15**: 4984−5001.

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First principles theory of phthalocyanines and corroles: From molecules to crystals

Leeor Kronik[a]

[a] *Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovoth 7610001, Israel*

The unique electronic and optical properties of phthalocyanines and corroles continue to be of much interest for a variety of applications. However, predicting these properties from first principles using density functional theory has often proven challenging. For molecules, severe self-interaction errors can arise due to localized metal-related orbitals. For crystals, one needs to address dispersive interactions, the description of multiple polymorphs, and the solid-state renormalization of energy levels due to dielectric screening. Here, I will present recent progress on these issues, as well as selected applications to important issues in contemporary experimental research of phthalocyanines and corroles.

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Enhanced proton pumping of cytochrome *c* oxidase in the presence of Higd1A

Minoru Kubo[a]

[a]*Graduate School of Science, University of Hyogo*

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Cytochrome *c* oxidase (CcO), the terminal enzyme of the mitochondrial respiratory chain, catalyzes the four-electron reduction of molecular dioxygen (O_2) to water using electrons supplied by cytochrome *c*. This redox reaction is tightly coupled to proton translocation across the mitochondrial inner membrane, generating the electrochemical proton gradient that drives ATP synthesis. In mammalian mitochondria, the efficiency and regulation of this energy-conversion process are modulated at multiple levels, including changes in cellular conditions, interactions with regulatory proteins, and alterations in subunit composition. In particular, hypoxic conditions induce a range of adaptive responses that modulate mitochondrial respiration, such as isoform switching of CcO subunits and the expression of hypoxia-responsive regulatory factors. Higd1A is a hypoxia-inducible membrane protein that has been implicated in the regulation of mitochondrial respiration and cellular energy homeostasis. Previous studies have reported that the presence of Higd1A correlates with enhanced CcO activity under hypoxic stress, suggesting a role in maintaining ATP production when oxygen availability is limited [1,2]. However, the specific functional consequences of Higd1A on individual steps of the CcO reaction, namely oxygen reduction and proton pumping, have remained unclear. In this study, we spectroscopically examined the influence of Higd1A on distinct functional aspects of CcO using a reconstituted liposome system. Purified mitochondrial CcO was incorporated into lipid vesicles in the presence or absence of Higd1A, allowing functional comparisons to be performed under *in vitro* conditions. The O_2 consumption and proton pumping rates of CcO were quantified separately using the reconstituted samples. Oxygen reduction was monitored by visible absorption spectroscopy employing hemoglobin as an O_2 indicator, whereas proton translocation was evaluated using phenol red as a pH-sensitive probe. These measurements revealed that the presence of Higd1A led to a pronounced acceleration of the proton pumping rate without a proportional increase in the rate of O_2 consumption. This implies an increase in the apparent H^+/e^- coupling efficiency, defined as the probability of proton translocation per electron transferred through CcO. In other words, Higd1A selectively enhances the proton-pumping efficiency of CcO rather than a simple acceleration of catalytic turnover. This finding provides a functional framework for understanding how hypoxia-induced regulatory factors can fine-tune mitochondrial respiration and is complementary to existing models of respiratory adaptation involving CcO isoform composition and supercomplex organization.

REFERENCES

1. T. Hayashi, et al., Higd1a is a positive regulator of cytochrome *c* oxidase. *Proc. Natl. Acad. Sci. USA* **112**, 1553–1558 (2015).
2. T. Nagao, et al., Higd1a improves respiratory function in the models of mitochondrial disorder. *FASEB J.* **34**, 1859–1871 (2020).

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π-Expanded BODIPYs for Applications in Photocatalysis and Photodetection

Yuji Kubo[a,b]

[a]*Department of Applied Chemistry, Graduate School of Urban Environmental Sciences, Tokyo Metropolitan University*
[b]*Research Center for Hydrogen Energy-based Society, Tokyo Metropolitan University*

The current demand for a feasible platform in energy conversion and optoelectronics has motivated us to develop π-expanded BODIPYs, which offer outstanding photophysical properties in the long-wavelength region. To this end, the fusion of aromatic rings at the [*a*]/[*b*] positions of the BODIPY core is an effective strategy to induce a longer-wavelength shift of the absorption band. Furthermore, adjustable photophysical properties and high photostability enable the application of ring-fused BODIPYs in light-harvesting materials. This lecture consists of two parts: the former focuses on advances in π-extended BODIPYs applicable to photocatalysis in green energy conversion [1]. Our interest in panchromatic sunlight energy harvesting, being one of the ultimate goals of an efficient photosensitizer, motivated us to investigate a benzo[*a*]-fused BODIPY and phenothiazine-based D–D'–π–A system (**1**) (Figure 1) [2]. The photophysical property leads to panchromatic absorption up to 780 nm when deposited on a Pt/hierarchical porous TiO_2 (HPT500). The resultant system, Pt/HTP500/**1**, exhibited excellent H_2 production in the presence of ascorbic acid when irradiated with $\lambda > 400$ nm light using a Xe lamp at an intensity of 100 mW cm^{-2}. A high turnover number of 11,100 and a turnover frequency of 1,110 h^{-1} were achieved for H_2 production after 10 h of irradiation. On the other hand, fusing the aromatic ring at the *b*-bond of the pyrrole unit is an efficient strategy to narrow the band gap owing to the stabilization of the LUMO energy level. Asymmetric BODIPY (**2**) composed of benzofuran[3,2-*b*]pyrrole and pyrromethene units was prepared for photocatalytic hydrogen production. [3] For the second topic, ring-fused BODIPYs have been applied to NIR photodetectors, which are useful in night vision, bioimaging, biometric authentication, etc. Considering the criteria that involve (1) absorption band with a high molar extinction coefficien and narrow full width at half maximum in the NIR region, (2) high carrier mobility, and (3) high photo and thermal stability, we prepared dibenzofuran[*a*]-fused BODIPYS with benzo[1,3,2]oxazaborinine unit (**3**) [4], which having an intense absorption band with a λ_{max} value of 812 nm ($\varepsilon = 1.3 \times 10^5$ M^{-1} cm^{-1}), as rationalized by time-dependent density functional theory (TD-DFT)/DFT calculations. Using a resistance-heating-type vacuum-deposition method, the rigid π-conjugated structure of **3** enabled its application as an NIR photodetector in a single-component device (indium tin oxide/**3**/Al). Current–voltage (*J*–*V*) measurements under photoirradiation at 870 nm (120 μW cm^{-2}) produced a photocurrent of 6.05×10^{-7} A cm^{-2} at a bias potential of 0.1 V. The obtained insight will facilitate the rational design of future NIR dyes tailored for specific applications.

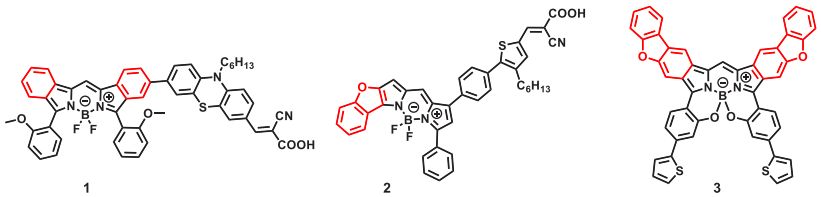


Figure 1. Chemical structures of dyes **1**–**3**.

REFERENCES

1. Y. Kubo, M. Ito, *ChemNanoMat*, **2026**, *12*, e202500559.
2. O. Suryani, Y. Higashino, H. Sato, Y. Kubo, *ACS Appl. Energy. Mater.*, **2019**, *2*, 448–458.
3. K. Makino, T. I, Y. Kubo, *Sustain. Energy Fuel.*, **2021**, *5*, 3676–3686.
4. A. Suzuki, R. Yamamoto, M. Ito, Y. Kubo, *ChemPlusChem*, **2025**, *90*, e202500021.

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Porphyrinoids as functional molecules for application in gas sensors

Abhishek Kumar[a], Marcel Bouvet[b], Charles Devillers[b], Mathilde Rieu[a]

[a] *Mines Saint-Etienne, Univ. Lyon, CNRS, UMR 5307 LGF, Centre SPIN, 158 cours Fauriel-42023 Saint-Etienne, France*

[b] *Institut de Chimie Moléculaire de l'Université de Bourgogne, UMR CNRS 6302,Université Bourgogne, 9 avenue Alain Savary, 21000, Dijon, France*

e-mail address: abhishek.kumar@emse.fr

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Surface functionalization is a promising approach to promote the specific interactions at the solid-gas interfaces. This strategy is being increasingly adopted to address the challenge of limited selectivity in gas sensors. Metal porphyrinoids (phthalocyanines and porphyrins) have been widely used in gas sensors in conjunction with different transducing modes, such as resistive, acoustic, optical, plasmonic and electrochemical. Such diverse use of porphyrinoids has been possible because of their multifunctional properties, like semiconducting nature, electrochemical activity, electronic interaction and enriched photophysics. Use of these macrocycles as a functional coating either on the gas sensor electrodes or on the sensing layer is although less explored. In this endeavor, the aim of my collaborative research activities is to develop functional coating of metal phathalocyanine and porphyrins on range of conducting surfaces and explore their application in conductometric gas sensors. In one typical approach, I am using diazonium electroreduction method to covalently graft porphyrins on gas sensors electrodes, such as ITO or gold and over the metal oxide sensing layer, such as tin oxide (SnO_2). In this method, the amino derivative of porphyrin is at first reacted by sodium nitrite in an oxygen free and acidic environment to produce the corresponding diazonium derivative (Fig. 1a). The application of a negative electrochemical potential produces a reactive porphyrin free radical at the electrode-solution interface, which is finally grafted on the surface. I am characterizing such grafting process by coupled characterization, such as electrochemical quartz chemical microbalance (EQCM), which monitors the mass deposition on the surface during the electrochemical grafting in terms of fundamental oscillating frequency shift of quartz (Fig. 1b). The EQCM measurements provide a direct proof of surface grafting and its quantification. Further investigation of electrografting mechanism and use of these modified surfaces in gas sensors are scopes of our ongoing works.

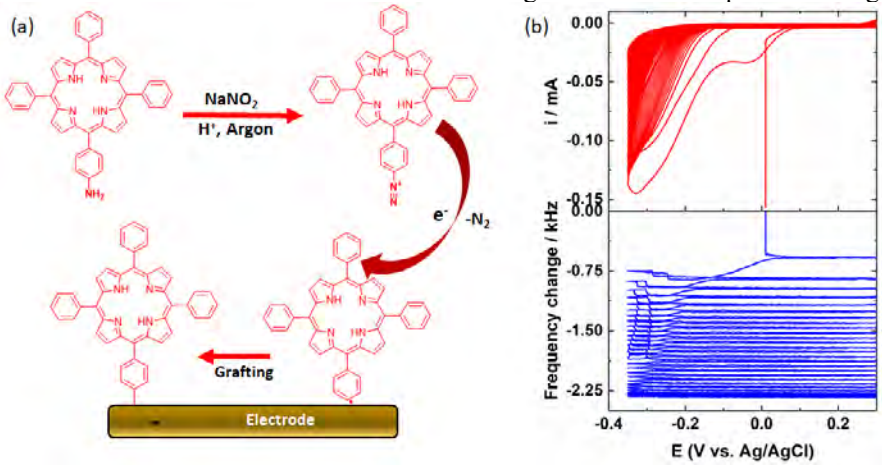


Figure 1: Schematic of electrografting of porphyrin by diazonium electroreduction (a). the variation of voltammograms and frequency shifts in the EQCM measurement associated to porphyrin electrografting (b).

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Efficient Synthesis of Heterocycle-Fused Porphyrins with Enhanced NIR Absorption and Singlet Oxygen Generation

Dalip Kumar

Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani Campus. Pilani-333031, Rajasthan, India ; E-mail: dalipk@pilani.bits-pilani.ac.in

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Porphyrins have gained significant interest in material and biomedicine research fields due to their special electronic and redox properties. Structural modification of porphyrin core enables π-conjugation over the macrocycle which causes a significant improvement in photophysical properties such as red-shifted absorption and efficient emission spectra towards the near IR region [1-2]. The π-extended porphyrins and loss of symmetry causes splitting in their energy levels in the π-π * levels, which reduces the band gap and results in the shifting and broadening of the Soret band, along with increase in the intensity of Q band. Particularly, heteroatom structural variation of porphyrin core has become an important milestone in porphyrin chemistry due to diversity in available heterocycles, and the presence of heteroatoms can act as an electron-donor/acceptor unit or provide an external coordination site for forming metal complexes. Further, integration of heteroaromatic systems into the porphyrin core increases co-planarity by incorporating the heteroatom into the extended π-system [2-3]. Therefore, in recent years, peripheral *N*-heterocycle-annulation of porphyrins (*meso-β*), (*β -β*) and *β-meso-β*) have been reported [4-5]. With immense usefulness of nitrogen-embedded π -extended porphyrins and our continued efforts to identify porphyrin-based novel photosensitizers [6-8] recently we have developed a facile and efficient protocol to access structurally diverse *N*-heterocycle-fused (*meso-β, β*-β) and appended porphyrins in good yields. Some of the prepared heterocycle-fused porphyrins exhibit red-shifted absorption, enhanced singlet oxygen generation, and respond to protonation and de-protonation processes to produce a switchable pH-sensitive near-IR chromophore. The developed synthetic protocol and photophysical studies of the prepared heterocycle porphyrins will be shared in the conference presentation.

REFERENCES

1. M. Pawlicki, H. A. Collins, R. G. Denning, H. L. Anderson, Angew. Chem. Int. Ed. 48, **2009**, 3244.
2. N. Fukui, W.-Y. Cha,.; S. Lee, S. Tokuji, D. Kim, H. Yorimitsu, A. Osuka, Angew. Chem. Int. Ed. 52, **2013**, 9728.
3. J. Akhigbe, M. Zeller, C. Bruuckner, Org. Lett. 13, **2011**, 1322.
4. M. Berthelot, G. Hoffmann, A. Bousfiha, J. Echaubard, J. Roger, H. Cattey, A. Romieu, D. Lucas, P. Fleurat-Lessard, C. H. Devillers, Chem. Commun. 54, **2018**, 5414.
5. P. Singh, M. Nath, Org. Lett. **2022**, 24, 8586
6. B. Kumar, S. B. Khandagale, N. Verma, T. P. Pandurang, E. Iype, D. Kumar, Org. Biomol. Chem. 20, **2022**, 7040.
7. N.Verma, S. B. Khandagale, E. Iype, N. Grover, D. Kumar, Eur. J. Org. Chem. 29, **2026**, e202501000.
8. P. P. Taur, N. Verma, D. Sharma, D. Kumar, J. Org. Chem. 90, **2025**, 10, 3570.

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Carbenaporphyrinoid Complexes of Coinage Metals and Zinc

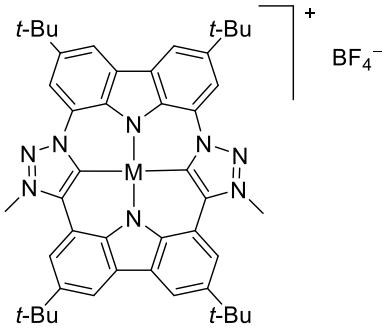
Doris Kunz, Benedikt Distel, Viola Munzert, Malín Moya Llasat, Theo Maulbetsch

Institut für Anorganische Chemie, University of Tübingen, Auf der Morgenstelle 16, 72076 Tübingen, Germany

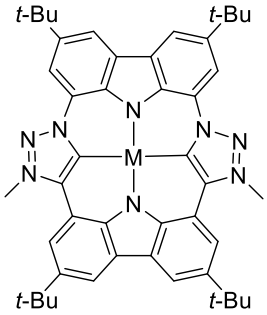
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The donor atoms in porphyrins can be modified by either replacing the pyrrol moieties with suitable heterocycles[1] or by formally rotating them under the formation of N-confused porphyrins.[2] The latter can be regarded as containing carbene donor atoms.[2c]
We have replaced two of the pyrrol moieties by triazolinylidenes, so-called mesoionic carbenes, in order to enhance the electron donor properties further. The resulting porphyrinoid ligand CTP would formally be an antiaromatic 20 electron π-system, but instead, we have shown that the individual aromatic character of the heterocycles is kept. The geometry of CTP complexes is surprisingly similar to the respective porphyrin complexes, while electronic differences are pronounced, which consequently affects their reactivity.[3]

To take advantage of the stronger ligand field of the CTP ligand, we will present the synthesis and the properties of coinage metal-CTP complexes in the formal oxidation state +III. In the case of Cu-CTP complexes, the paramagnetic Cu^{II}(CTP) complex can also be isolated. With Zn^{2+}-precursors an unexpected rich coordination chemistry was found and investigated including dinuclear complexes as well as the mononuclear complex [Zn(CTP)].



[M(CTP)]BF_4
(M = Cu, Ag, Au)



[M(CTP)]
(M = Cu, Zn)

REFERENCES

1. a) L. Arnold, M. Baumgarten, K. Müllen, *Chem. Commun.* **2012**, *48*, 9640-9642; b) C. Maeda, M. Masuda, N. Yoshioka, Org. Lett. 2013, 15, 3566-3669.
2. a) H. Furuta, T. Asano, T. Ogawa, *J. Am. Chem. Soc.* **1994**, *116*, 767-768; b) P. J. Chmielewski, L. Latos-Grażyński, K. Rachlewicz, T. Glowiak, *Angew. Chem. Int. Ed. Engl.* **1994**, *33*, 779-781; c) A. Ghosh, *Angew. Chem. Int. Ed. Engl.* 1995, 34, 1028-1030.
3. T. Maulbetsch, D. Kunz, *Angew. Chem. Int. Ed.* **2021**, *60*, 2007-2012.

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Photothermal therapy with Nano-dICG and the role of immune response at murine melanoma model

Cristina Kurachi[a], Letícia P Martinelli[a], Layla Pires[b], Gang Zheng[b], Brian Wilson[b]

[a]*University of Sao Paulo, Sao Carlos, Sao Paulo, Brazil*
[b]*University Health Network, Toronto, Ontario, Canada*

Melanoma, even with the advances in immunotherapy, still presents high morbidity and mortality rates due to its aggressive behavior and poor response to available treatment modalities [1]. Photodynamic therapy (PDT) and photothermal therapy (PTT) are potential treatment options in Oncology, but with limited volumetric response due to the light penetration within biological tissues [2]. Solid highly pigmented tumors, as melanomas, are relevant challenges for any photonic technique. Nano-dICG is a nanoemulsion presenting a highly stable and potent photothermal agent based on the dimeric form of indocyanine green [3]. The efficiency of the PTT using nano-dICG for the treatment of cutaneous melanoma was evaluated in a murine model. B16F10-Luc2 cells were intradermally injected and tumors treated when reached 2-3 mm of thichkness. Intratumoral and intravenous administration of nano-dICG, distinct irradiance and fluence levels at 808 nm irradiation, at immunocompromised and immunocompetent animals were investigated. Photoacoustic/fluorescence imaging was used to determine best drug-light intervals for the intravenous photosensitizer administration. Bioluminescence imaging, immunohistochemistry analysis (H&E, S100, Ki67) and survival curves were analyzed as treatment response. Rechallenge assay injecting melanoma cells through the tail vein was performed in animals showing complete tumor eradication at 30 days after PTT. As most relevant result, tumor eradication at 30 days after PTT, and no development of melanomas after rechallenge assay in all animals (n=12) was achieved at 1-hour and 6-hour DLI groups of the immunocompetent animals. In the immunocompromised animals, the best treatment protocol resulted in 67% of disease-free Kaplan Meier curve at 30th day. Partial tumor response was achieved at the groups that received laser irradiation without nano-dICG administration, due to the high concentration of melanin, but tumor regrowth and shorter survival were observed. In conclusion, our results showed strong evidence that nano-dICG-PTT mediated activation of the immune system resulting in eradication of cutaneous melanoma up to 3 mm of thickness and adaptative immune response at 30th day after primary tumor treatment. The activation of the immune response by PTT may represent an important feature to overcome the lack of therapeutic response in highly pigmented tumors.

REFERENCES

1. Tasdogan, A.; Sullivan, R.J.; Katalinic, A.; Lebbe, C.; Whitaker, D.; Puig, S.; Poll-Franse, L.V.; Massi, D.; Schadendorf, D. Cutaneous melanoma. Nature Reviews disease primers, **2025**, 11:23. https://doi.org/10.1038/s41572-025-00603-8.
2. Pires, L.; Demidov, V.; Wilson, B. C.; Salvio, A. G.; Moriyama, L.; Bagnato, V. S.; Vitkin, I. A.; Kurachi, C. Dual-Agent Photodynamic Therapy with Optical Clearing Eradicates Pigmented Melanoma in Preclinical Tumor Models. *Cancers* **2020**, *12* (7), 1–17. https://doi.org/10.3390/cancers12071956.
3. Kwon, N.; Jasinevicius, G. O.; Kassab, G.; Ding, L.; Bu, J.; Martinelli, L. P.; Ferreira, V. G.; Dhaliwal, A.; Chan, H. H. L.; Mo, Y.; Bagnato, V. S.; Kurachi, C.; Chen, J.; Zheng, G.; Buzzá, H. H. Nanostructure-Driven Indocyanine Green Dimerization Generates Ultra-Stable Phototheranostics Nanoparticles. *Angewandte Chemie - International Edition* **2023**, *62* (28). https://doi.org/10.1002/anie.202305564.

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Mechanistic Role of the Excited Triplet State of Zn(II) Porphyrin in Photocatalytic Carbon Dioxide Reduction

Yusuke Kuramochi[a]

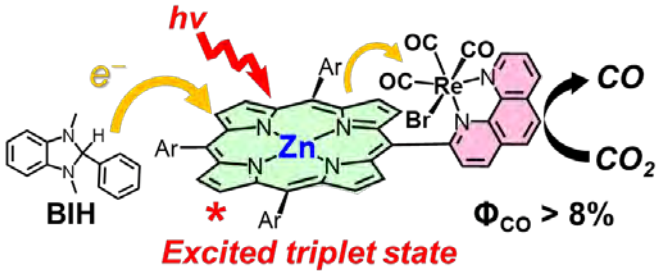
[a]*Department of Science, Faculty of Science and Engineering, Kindai University*

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Zinc(II) porphyrins have long been studied as synthetic models of chlorophyll and bacteriochlorophyll in natural photosynthesis, and their strong visible-light absorption has led to extensive investigations focusing primarily on the reactivity of their excited singlet states. In particular, singlet-singlet energy transfer and the singlet-driven photoinduced electron transfer have been widely explored as key processes in artificial photosynthetic systems. In contrast, intersystem crossing from the excited singlet state to the excited triplet state of porphyrin has often been regarded as an undesirable process in photosynthetic model systems, because excited triplet states are inefficient for long-range energy transfer and may act as energy traps or quenching sites.

However, this perspective is fundamentally different in photocatalytic reactions that rely on diffusion-controlled intermolecular electron transfer. In such systems, electron transfer requires molecular encounters by diffusion, which occur on much longer timescales than intramolecular processes, and therefore demand long-lived excited states to maintain productive reactivity. Accordingly, the excited singlet state and the charge-separated state formed by the singlet-driven intramolecular photoinduced electron transfer are intrinsically short-lived and unsuitable for diffusion-controlled intermolecular electron transfer, whereas the excited triplet state is long-lived and ideally suited for photocatalytic redox processes.

Here, the present work demonstrates that the excited triplet state of Zn(II) porphyrin plays a decisive and constructive role in photocatalytic CO_2 reduction.[1,2] The Zn(II) porphyrin and the Re(diimine)$(CO)_3$ complex, which serves as a CO_2 reduction catalyst, were directly linked in a geometry in which the porphyrin plane and the diimine ligand are arranged perpendicular to each other (Figure). This structural arrangement enhances intersystem crossing of the porphyrin via the heavy-atom effect of the Re center, thereby selectively populating the triplet state of the porphyrin. The resulting long-lived excited triplet state efficiently accepts an electron from 1,3-dimethyl-2-phenyl-2,3-dihydro-1*H*-benzo[*d*]imidazole (BIH) used as an electron donor, and subsequently transfers the electron to the Re catalyst. The electron transfer mediated through the excited triplet state of Zn(II) porphyrin is evidenced by quenching the Re-induced room-temperature phosphorescence of the porphyrin by BIH,[1] as well as by transient absorption and time-resolved infrared spectroscopy.[3] In this presentation, in addition to these phenomena, the photophysical properties and catalytic activities of a series of photocatalytic systems in which the linkage positions between the Zn(II) porphyrin and the Re(diimine)$(CO)_3$ complex are systematically varied will also be introduced.



REFERENCES

1. Y. Kuramochi, Y. Fujisawa, A. Satake, *J. Am. Chem. Soc*. **2020**, *142*, 705.
2. Y. Kuramochi, Y. Suzuki, S. Asai, T. Suzuki, H. Iwama, M. S Asano, A. Satake, *Chem. Sci.* **2023**, *14*, 8743.
3. T. Honda, T. Ehara, R. Sato, T. Ogawa, Y. Kuramochi, A. Satake, K. Miyata, K. Onda, *Inorg. Chem.* **2024**, *63*, 23524.

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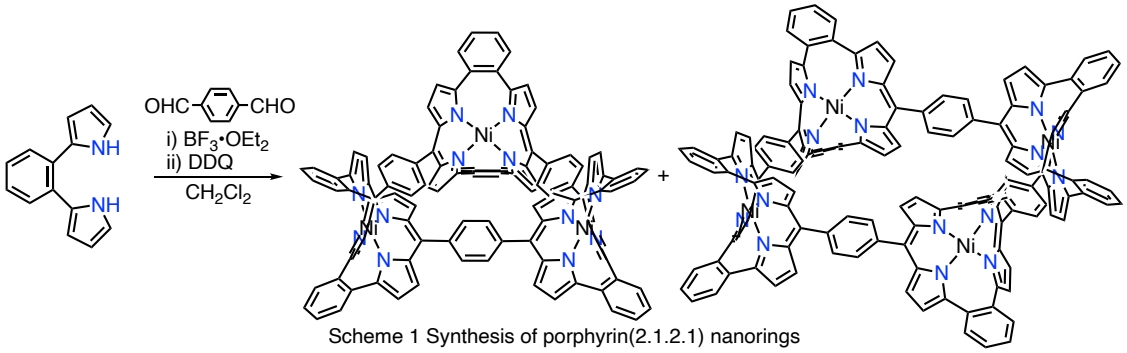


Syntheses of Expanded Porphyrins from *o*-Diarylbenzenes and 3,4-Diarylmaleimides

Daiki Kuzuhara[a], **Ryoma Matsuura**[a], **Anji Ohta**[a]

[a] *Faculty of Science and Engineering, Iwate University*

The creation of expanded porphyrins is of significant importance to the field of porphyrin chemistry, and as such, should be given due consideration in any investigation of this area. In the field of expanded porphyrins, our research group has made contributions to the synthesis of this class of compounds. Our studies have led to the development of a novel synthesis method for expanded porphyrins, which consists of a linker consisting of two carbon atoms connecting pyrrole units. Porphyrin(2.1.2.1) is classified as a member of the porphyrin family, characterized by a structural configuration comprising two dipyrrin units and two *o*-phenylene bridges. Porphyrin(2.1.2.1) can be synthesized through an acid-catalyzed condensation of *o*-di(pyrrol-2-yl)benzene and aryl aldehydes[1]. Porphyrin(2.1.2.1) forms deeply saddle-shaped molecular structures. This distinctive non-planar configuration finds application in the construction of porphyrin nanobelts from 1,2,4,5-tetra(pyrrol-2-yl)benzene and aryl aldehydes[2]. Furthermore, we have synthesized *p*-phenylene linked porphyrin(2.1.2.1) nanorings *via* acid-catalyzed condensations of *o*-di(pyrrol-2-yl)benzene and terephthalaldehyde (Scheme 1). In addition, porphyrin(2.1.2.1) is employed as a metal ligand in a manner analogous to general porphyrins for synthesizing various metal complexes. *o*-Di(pyrrol-2-yl)benzene and its derivatives also possess the potential to function as intermediates in the creation of expanded porphyrins and related compounds. Di(pyrrol-2-yl)phthalimide was utilized as a starting material to yield calix[4]pyrrole and calix[6]pyrrole during a condensation reaction with acetone. Calix[*n*]bispyrrolyphthalimides selectively recognize fluoride anions, resulting in clear color changes that can be observed by the naked eye. This is due to the pyrrole and phthalimide groups acting as donor and acceptor, respectively. Conversely, 3,4-di(pyrrol-2-yl)maleimide exhibited divergent reactivity. Despite an unsuccessful attempt to isolate porphyrin(2.1.2.1) under the standard conditions of the condensation reaction, oxidized compounds were successfully isolated. In this presentation, the recent progress made in synthesizing expanded porphyrins from *o*-di(pyrol-2-yl)benzene and 3,4-di(pyrol-2-yl)maleimide derivatives will be discussed.



Scheme 1 Synthesis of porphyrin(2.1.2.1) nanorings

REFERENCES

1. D. Kuzuhara, W. Furukawa, A. Kitashiro, N. Aratani, H. Yamada, *Chem. Eur. J.* **2016**, *22*, 10671–10678.
2. S. Xue, D. Kuzuhara, N. Aratani, H. Yamada, *Org. Lett*. **2019**, *21*, 2069-2072.

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Bowl-to-bowl inversion in Subphthalocyanines

Jorge Labella[a,b], **Marta Gómez-Gómez**[a] **Tomás Torres**[a,c,d]

[a]*Organic Chemistry Department, Universidad Autónoma de Madrid, 28049, Madrid, Spain*
[b]*Department of Molecular Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan*
[c]*IMDEA-Nanociencia, c/Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain*
[d]*Institute for Advanced Research in Chemical Sciences, Campus de Cantoblanco, 28049 Madrid, Spain*

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Bowl-shaped aromatics have emerged as powerful scaffolds in the field of π-conjugated materials due to their disruptive, topology-driven properties. A hallmark of these systems is the bowl-to-bowl (*BtB*) inversion—a fluxional process that interconverts the concave and convex faces, compromising the configurational stability of enantiopure derivatives.[1] This is especially critical for designing chiral materials, where even minimal enantiomeric erosion can severely impact performance. In boron subphthalocyanines (SubPcs)—arguably the most versatile bowl-shaped aromatics in materials science—this inversion is typically locked by the tetrahedral boron center. [2] However, axial ligand removal renders *BtB* inversion conceptually accessible.

Herein we show that the *BtB* inversion of SubPcs can be indeed experimentally observed using enantiopure derivatives as stereochemical probes.[3] By combining both on-surface and solution-phase chemistry with theoretical calculations, we elucidate the conditions under which this process occurs, as well as the underlying mechanisms involved. Moreover, the electronic, chemical and steric aspects governing this process are analyzed, and practical guidelines to preserve the enantiopurity of SubPcs are provided.

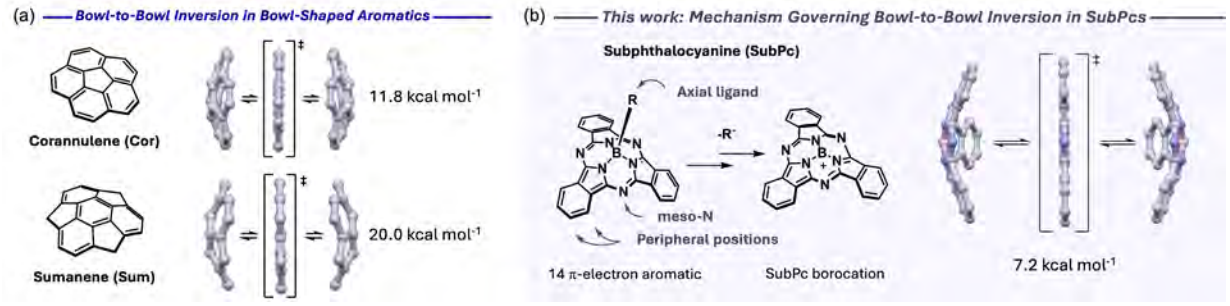


Figure 1. (a) *BtB* inversion of representative bowl-shaped aromatics. (b) Illustration of the *BtB* inversion of the SubPc borocation upon removal of the axial ligand. The energy barriers indicated in each case were calculated by DFT at the B97D3/6-31G** level of theory. Hydrogen atoms have been omitted for clarity from the ball-and-sticks models.

REFERENCES

1. Saito, M.; Shinokubo, H; S. Hidehiro. *Mater. Chem. Front.* **2018**, *2*, 635–661.
2. Labella, J; Torres, T. *Trends Chem.* **2023**, *5*, 353–366.
3. Gómez-Gómez, M; Labella, J; Torres, T. *Submitted.*

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NMR Detection of Enantiomeric Excess Using Symmetric Porphyrins as Prochiral Solvating Agents (*pro*-CSAs)

Jan Labuta

Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Tsukuba, Japan (Labuta.Jan@nims.go.jp)

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More than half of the drugs currently in use are chiral compounds, and in recent years nearly 90% of newly approved chiral drugs have been launched as single enantiomers rather than racemic mixtures. While enantiomers share the same chemical composition, they often display different pharmacological, toxicological, and metabolic properties. Variations in enantiomeric composition can critically influence efficacy, safety, and dosage requirements. Thus, precise control and monitoring of chirality are cornerstones of modern pharmaceutical development and clinical application.

There are three standard protocols for measuring enantiomeric excess (*ee*) using nuclear magnetic resonance (NMR) spectroscopy. However, these are always based on the formation of diastereomers in solution. We have developed an NMR sensing method utilizing prochiral porphyrin derivatives (an example is shown in Fig.1a) as detectors of analytes' enantiomeric excess (*ee*). In this method, the formation of diastereomers is not required (Fig.1b), and the *ee* is obtained from the detector's NMR spectrum as the magnitude of splitting $\Delta\delta$ of the reporting group (Fig.1c), which has a fundamental linear dependence on *ee* (Fig. 1d) [1-5]. Based on symmetry requirements, we also tested the *pro*-CSA mechanism on small systems, such as benzylamine (prochiral detector) with 2-phenoxylpropionic acid (analyte) [6] or salen-Zn_2 coordination complex (prochiral detector) with 2-phenoxylpropionic acid (analyte) [7]. The mechanism, stoichiometric effects, drawbacks, and potential applications of the *pro*-CSA sensing method will be discussed.

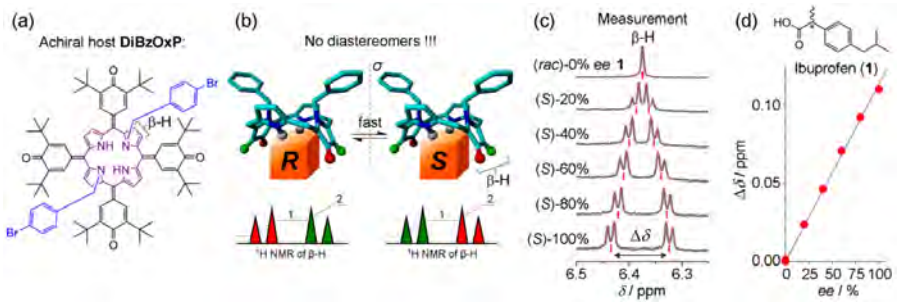


Fig. 1. (a) Structure of prochiral porphyrin derivative **DiBzOxP**. (b) Schematic illustration of the sensing mechanism. (c) NMR spectra of porphyrin β-H reporting group in the presence of various *ee* of ibuprofen (**1**) analyte. (d) Fundamental linear relationship between induced chemical shift non-equivalency $\Delta\delta$ and *ee* as obtained from (c).

REFERENCES

1. A. Shundo, J. Labuta, J. P. Hill, S. Ishihara, and K. Ariga. *J. Am. Chem. Soc.* **2009**, *131*, 9494.
2. J. Labuta, S. Ishihara, A. Shundo, S. Arai, S. Takeoka, K. Ariga, and J. P. Hill. *Chem. Eur. J.* **2011**, *17*, 3558.
3 J. Labuta, S. Ishihara, T. Šikorský, Z. Futera, A. Shundo, L. Hanyková, J. V. Burda, K. Ariga, and J. P. Hill. *Nat. Commun.* **2013**, *4*, 2188.
4. J. Labuta, J. P. Hill, S. Ishihara, L. Hanyková, K. Ariga. *Acc. Chem. Res.* **2015**, *48*, 521**.**
5. J. Labuta, S. Ishihara, J. P. Hill. *J. Porphyrins Phthalocyanines* **2020**, *24*, 320.
6. S. Ishihara, J. Labuta, Z. Futera, S. Mori, H. Sato, K. Ariga, J. P. Hill. *J. Phys. Chem. B* **2018**, *122*, 5114.
7. K. Takimoto, S. Ishihara, J. Labuta, V. Březina, D. T. Payne, J. P. Hill, K. Ariga, M. Sumita, S. Mori, H. Sato. *J. Phys. Chem. Lett.* **2020**, *11*, 8164.

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Biosynthesis of the Cobalamin Lower Base

Andrew Lawrence[a]

[a]*School of Biological Sciences, University of Southampton, Southampton, SO17 1BJ, United Kingdom.*

Cobalamin (vitamin B_{12}) is a structurally complex metallocofactor whose biological function is strongly influenced by the identity of its lower axial ligand. While the aerobic route to the canonical lower base 5,6-dimethylbenzimidazole (DMB) has been well described; the anaerobic pathway has remained comparatively enigmatic despite its widespread distribution among bacteria and archaea. This presentation will focus on recent advances in elucidating the anaerobic biosynthesis of the cobalamin lower base.

I will describe the identification and structural characterization of previously unrecognized pathway intermediates that define a distinct, oxygen-independent route to DMB formation. Central to this pathway are two cobalamin-associated radical S-adenosyl-L-methionine (rSAM) enzymes, whose functions and substrate specificities we have now characterized biochemically and mechanistically. Together, these findings provide a revised framework for anaerobic lower base biosynthesis and clarify how radical SAM chemistry has been adapted to construct one of the most distinctive features of cobalamin.

More broadly, this work highlights how variation in lower ligand biosynthesis contributes to cobamide diversity, metabolic specialization, and ecological adaptation in anaerobic microorganisms

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Radical SAM enzymes in heme and heme d_1 biosynthesis

Gunhild Layer, Anika Guther and Sam Washington

University of Freiburg, Institute of Pharmaceutical Sciences, Pharmaceutical Biology

Heme and heme d_1 are both naturally occurring, iron-containing tetrapyrroles. While heme fulfils a variety of different functions in almost all living organisms, heme d_1 is restricted to some denitrifying bacteria. Structurally, heme belongs to the metalloporphyrins, while heme d_1 is a metalated isobacteriochlorin. Besides the differences in their macrocycle core structures, heme and heme d_1 also display individual patterns of tetrapyrrole side chains. Despite these structural differences, the biosynthetic pathways to heme and heme d_1 share some common steps and intermediates [1]. In archaea and sulfate-reducing bacteria, heme is synthesized by the siroheme-dependent (SHC) pathway *via* the intermediates siroheme, 12,18-didecarboxy-siroheme (DDSH), and iron-coproporphyrin III (Fe-Copro) [2]. Heme d_1 is also derived from siroheme *via* DDSH, 3,8-dideoxo-dihydroheme d_1 (DDDH), and dihydro-heme d_1 [2, 3]. Therefore, the last common intermediate of the SHC pathway to heme and the biosynthesis route to heme d_1 is DDSH.

Interestingly, the conversion of DDSH to either Fe-Copro during heme biosynthesis or DDDH during heme d_1 biosynthesis is catalyzed by two related enzymes, AhbC and NirJ, respectively. Both proteins belong to the family of radical *S*-adenosyl-L-methionine (SAM) enzymes and share about 17 % amino acid sequence identity [3]. As both enzymes accept the same substrate but convert it into different products, it is intriguing to investigate how AhbC and NirJ achieve reaction specificity. For this purpose, the purified, recombinant enzymes are employed in enzyme activity assays showing the conversion of DDSH to Fe-Copro by AhbC and to DDDH by NirJ *in vitro*. Based on computational structural models of NirJ and AhbC, enzyme variants carrying amino acid exchanges within the putative active sites are generated and tested for enzymatic activity. Based on these biochemical experiments in combination with structure predictions, the reaction specificity of AhbC and NirJ will be discussed.

REFERENCES

1. Dailey H.A., Dailey T.A., Gerdes S., Jahn D., Jahn M., O'Brian M.R. & Warren M.J. (2017) Prokaryotic heme biosynthesis: Multiple pathways to a common essential product. *Microbiol. Mol. Biol. Rev.*, 81, e00048-16.
2. Bali S., Lawrence A.D., Lobo S.A., Saraiva L.M., Golding B.T., Palmer D.J., Howard M.J., Ferguson S.J. & Warren M.J. (2011). Molecular hijacking of siroheme for the synthesis of heme and d_1 heme. *Proc. Natl. Acad. Sci. USA*, 108, 18260–18265.
3. Meyer H., Hoock M.H., Zwara K., Jahn S., Schünemann V. & Layer G. (2025) The radical SAM enzyme NirJ cleaves off two propionate side chains with the release of acrylate during heme d_1 biosynthesis. *FEBS J.*, 292, 5151-5167.

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Stabilization and Characterization of a Heme-HNO Adduct in a Model Complex for Cytochrome P450nor

Nicolai Lehnert,[a] Daniel G. Castella,[a] Elizabeth C. Manickas[a]

[a]*University of Michigan, Department of Chemistry and Department of Biophysics, Ann Arbor, MI 48109-1055, USA (email: lehnertn@umich.edu)*

Denitrification is a microbial pathway in the nitrogen cycle that uses nitrate and nitrite as the terminal electron acceptors in respiration. Denitrifying bacteria and fungi efficiently detoxify the toxic metabolite nitric oxide (NO) of this process through reduction to nitrous oxide (N_2O) using nitric oxide reductase (NOR) enzymes. In fungi, for example *Fusarium oxysporum*, NO is reduced by a Cytochrome P450 type enzyme, called Cyt. P450nor.[1] This enzyme contains a heme *b* center coordinated to a proximal cysteinate ligand in the active site. In the proposed mechanism of Cyt. P450nor, the ferric heme binds NO first to form a ferric heme-nitrosyl complex, which is subsequently reduced by NAD(P)H to generate the key intermediate of the reaction, called Intermediate *I*. This species either corresponds to the Fe(II)-NHO adduct, or the corresponding, protonated species of Fe-NHOH type with unknown electronic structure. Intermediate *I* then reacts with the second equivalent of NO to form N_2O.

In order to obtain further insight into the nature of Intermediate *I*, we used a bulky bis-picketfence porphyrin, H_2[3,5-Me-BAFP], to generate the heme-HNO model complex [Fe(3,5-Me-BAFP)(MI)(NHO)] and study its electronic structure, and importantly, reactivity with NO. This complex can be cleanly generated at -30 ºC by reaction of [Fe(3,5-Me-BAFP)(MI)(NO)](OTf) with 1 equiv of [TBA](BH4). Under these conditions, the heme-HNO complex has a lifetime of about 1 hour, which allowed for a detailed spectroscopic characterization of this species.[2] The reactivity of the HNO complex with NO gas was assessed by quantitative gas headspace IR spectroscopy, and it was determined that this complex can in fact mediate N_2O formation by addition of NO gas. These results demonstrate that heme-HNO complexes are competent intermediates in Cyt P450nor.

To further our understanding of Intermediate *I*, we sought to increase the stability of our model complex by incorporating hydrogen bonding groups into the second coordination sphere (SCS). We synthesized a new asymmetric derivative of our scaffold, H_2[(3-NH_2)(3,5-Me)$_3$BAFP] and generated the corresponding ls-{FeNO}^{6} complex, [Fe((3-NH_2)(3,5-Me)$_3$BAFP)(NO)](OTf). Notably, this complex seems to bind one of the distal amine groups of the porphyrin scaffold to the sixth co-ordination site of the iron center. Treatment of this complex with a hydride donor then allows for the generation of [Fe((3-NH_2)(3,5-Me)$_3$BAFP)(NHO)], and the subsequent characterization of this complex with ^{1}H-NMR, UV-vis, and IR spectroscopy to evaluate its geometric and electronic structure. DFT calculations are further used to assess the effect of the SCS groups on the stability of heme-HNO adducts.

REFERENCES

1. Lehnert, N.; Kim, E.; Dong, H. T.; Harland, J. B.; Hunt, A. P.; Manickas, E. C.; Oakley, K. M.; Pham, J.; Reed, G. C.; Sosa Alfaro, V. *Chem. Rev.* **2021**, *121*, 14682-14905.
2. Manickas, E. C.; LaLonde, A. B.; Hu, M. Y.; Alp, E. E.; Lehnert, N. *J. Am. Chem. Soc.* **2023**, *145*, 23014-23026.

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Rigid expanded porphyrinoids: design, synthesis, and properties study

Chuanhu Lei[a]

[a]*Center for Supramolecular Chemistry and Catalysis, Department of Chemistry, College of Science, Shanghai University, Shanghai, 200444, China*

The continuous advancement of supramolecular chemistry is being driven by the design and synthesis of novel macrocyclic molecules. As a crucial category of macrocycles, expanded porphyrinoids not only play significant roles in fundamental research, such as aromaticity studies, coordination chemistry, and organic radicals, but also show promising potential in practical applications. For example, they are widely utilized as near-infrared absorbing dyes and photosensitizers to enhance the therapeutic effects of X-ray irradiation on tumors. Despite substantial progress in expanded porphyrinoid chemistry in recent years, their synthesis yield still tends to be low, and separation remains relatively challenging. Furthermore, the functionality of classic expanded porphyrinoids, composed of more than four pyrrole units, is relatively limited, necessitating further enrichment and expansion for diverse applications.

Based on this, we have proposed the concept of "balancing rigidity and flexibility" in molecular design. The aim is to enhance the rigidity of expanded porphyrinoids by incorporating rigid precursors. This approach resolves the challenge of generating numerous isomers due to structural flexibility during cyclization. Moreover, the introduction of conformational rigidity may unveil novel functionalities not found in traditional expanded porphyrinoids. In this presentation, we will discuss the successful construction of a series of expanded porphyrinoids guided by this strategy. In particular, we will highlight their outstanding properties, including chiroptical and distinctive photophysical properties that arise from their relatively stable conformations.[1-5]

REFERENCES

1. Han, P.; Duan, Z.; Shao, M.; Sessler, J. L.; Lei, C. *Angew. Chem., Int. Ed.* **2025**, *64*, e202413962.
2. Liang, K.; Chen, H.; Wang, X.; Lu, T.; Duan, Z.; Sessler, J. L.; Lei, C. *Angew. Chem. Int. Ed.* **2023**, *62*, e202212770.
3. Chen, H.; Lei, Y.; Xu, Y.; Shao, M.; Duan, Z.; Lei, C. *J. Org. Chem.* **2023**, *88*, 11352.
4. Zheng, Y.; Wang, X.; Chen, H.; Lu, T.; Duan, Z.; Lei, C. *Org. Lett.* **2022**, *24*, 2509.
5. Chen, H.; Shi, X.; Lun, Y.; Xu, Y.; Lu, T.; Duan, Z.; Shao M.; Sessler, J. L.; Yu, H.; Lei, C. *J. Am. Chem. Soc.* **2022**, *144*, 8194.

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Silicon Phthalocyanines: From Air Stable N-Type To Record Breaking P-Type Performance In OTFTs

Benoît H. Lessard[a,b]

[a]*Department of Chemical and Biological Engineering, University of Ottawa, 161 Louis Pasteur, Ottawa, Ontario K1N 6N5, Canada.*
[b]*School of Electrical Engineering and Computer Science, University of Ottawa, 800 King Edward Ave. Ottawa, Ontario K1N 6N5, Canada.*

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Silicon phthalocyanines (SiPcs) are a distinctive and underexplored class of phthalocyanines in which axial ligation at the silicon center provides unusual control over both molecular and solid-state properties. In contrast to metal-centered phthalocyanines, axial substitution in SiPcs enables systematic tuning of solubility, intermolecular interactions, and thin-film organization without substantially altering the macrocycle's electronic structure or optical absorption. This decoupling of molecular packing from frontier orbital energies makes SiPcs a powerful platform for establishing clear structure–property relationships.

Organic thin-film transistors (OTFTs) based on SiPcs demonstrate that axial group chemistry directly governs key device parameters. For example, increasing the electron-withdrawing character of the axial substituents systematically reduces threshold voltages over nearly an order of magnitude while maintaining electron mobilities exceeding 0.5 $cm^2\ V^{-1}\ s^{-1}$, among the highest reported for phthalocyanines[1]. More recently, siloxane-based functionalization strategies have enabled SiPcs that exhibit unipolar p-type transport with hole mobilities greater than 1 $cm^2\ V^{-1}\ s^{-1}$[2,3]. Together, these results show how targeted chemical modifications at the silicon center translate directly into quantifiable and tunable electronic responses.

To systematically link molecular structure, processing conditions, and device behavior, we employ high-throughput fabrication and characterization approaches that enable rapid exploration of the multidimensional parameter space associated with organic semiconductors. Using automated, on-chip fabrication of OTFTs, we map the influence of deposition parameters such as solvent evaporation rate, print speed, and substrate temperature across multiple SiPc derivatives, establishing clear correlations between processing conditions, thin-film morphology, molecular packing, and charge transport [4]. Extending this high-throughput philosophy to operational stability, we apply cyclic bias-stress testing protocols that enable statistically meaningful evaluation of environmental and operational effects over extended time scales [5].

Taken together, these results position silicon phthalocyanines as a chemically tractable platform where deliberate molecular design enables control over solid-state organization, processing behavior, and electronic function, providing a clear framework for linking synthesis to device-relevant properties.

REFERENCES

1. Advanced Functional Materials, 2024, 2408779
2. Advanced Functional Materials, 2025, e14609
3. Materials Chemistry Frontiers, 2025, 9, 3559-3571
4. Advanced Electronic Materials, 2025, 2400500
5. Small Methods, 2025, e00782

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Tuning Photosensitizer Performance: Spectroscopic Insights into *m*-THPC Interactions with Proteins, Micelles, and Graphene-Based Nanomaterials

Anna Lewandowska-Andralojc[a], Aleksander Kolman[a], Blazej Scheibe[b]

[a]*Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznanskiego 8, 61-614 Poznan, Poland*
[b]*NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, 61-614 Poznan, Poland*

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Meta-tetra(hydroxyphenyl)chlorin (*m*-THPC) is a highly efficient photosensitizer for photodynamic therapy (PDT), yet its strong aggregation in aqueous media severely limits singlet oxygen generation and therapeutic efficacy. This lecture presents spectroscopic insights into how the aggregation and excited-state deactivation pathways of *m*-THPC and related chlorins can be controlled through interactions with biological and nanostructured carriers. We demonstrate that complexation with bovine serum albumin (BSA) effectively suppresses aggregation, restores monomeric photophysics, and significantly enhances singlet oxygen quantum yield [1]. We then extend this concept to hybrid nanocarrier systems based on Pluronic P123 micelles and graphene oxide (GO) or reduced graphene oxide (RGO) (Fig. 1). Micellar encapsulation preserves the monomeric state of *m*-THPC, improves dispersibility in PBS, and enables efficient singlet oxygen production. In contrast, incorporation of GO induces strong fluorescence quenching and suppresses triplet-state formation via ultrafast photoinduced electron transfer, leading to reduced PDT activity but simultaneously introducing efficient photothermal conversion under near-infrared irradiation. By fine-tuning GO content, partial retention of photodynamic activity can be achieved alongside a robust photothermal response, enabling dual-mode PDT/PTT functionality within a single nanoplatform [2-3].

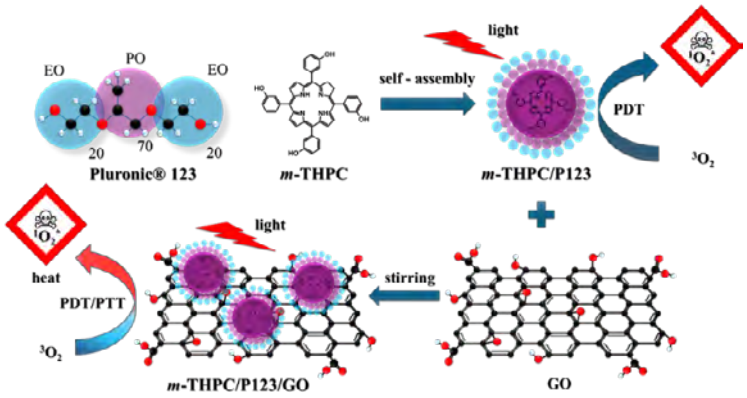


Fig. 1. Illustration of the ternary m-THPC/Pluronic P123/GO hybrid system for combined PDT/PTT therapy.

REFERENCES

[1] A. Kolman, T. Pedzinski, A. Lewandowska-Andralojc, *Sci. Rep*., 2024, 14, 22343
[2] A. Lindner, A. Lesniewicz, A. Kolman, D. Larowska-Zarych, B. Marciniak, A. Lewandowska-Andralojc, *J. Mat. Chem C*, 2024, 12 9012
[3] A. Kolman, B. Scheibe, A. Lewandowska-Andralojc, *J. Photobiol. Photochem. A*, 2026, 473, 116881

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Early transition-metal and f-block phthalocyanines: From colour tuning to catalysis

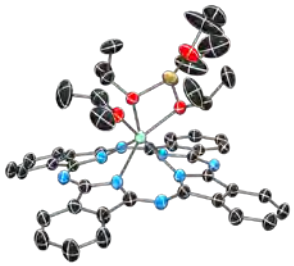
Daniel B. Leznoff[a]

[a] *Department of Chemistry, Simon Fraser University, Burnaby, Canada*

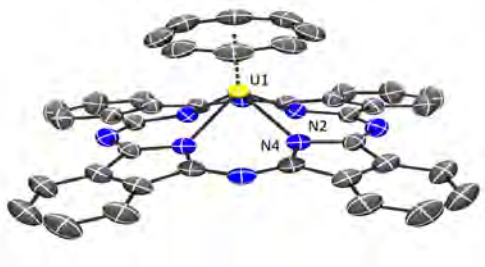
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Metallophthalocyanines (PcM) are highly industrially important, intensely coloured macrocyclic metal complexes that have a wide range of applications and are experiencing a 21st century Renaissance. Although there are PcM complexes reported for most metals in the periodic table, in practice most research has focused on late-transition metals. On the other hand, there are far fewer examples of phthalocyanines with early-transition and f-block metals - despite the rich organometallic-type reactivity of these metals - and thus we targeted new PcM complexes in this underdeveloped area of the periodic table. Given their larger ionic size, the unusual structural feature of the metal centre protruding far out of the Pc cavity is often prevalent. Hence, the exposure of the coordination sphere of these Lewis-acidic (often d^0) metals makes these PcM complexes attractive catalysts; this cis-oriented axial ligation also drastically improves the solubility, despite the Pc-ring remaining unsubstituted.

In this presentation the synthesis, properties and structural characterization of new PcM materials with M = zirconium, niobium, molybdenum, manganese and f-elements will be described. PcM complexes can be successively reduced using chemical, electrochemical, or photochemical methods to give rise to species containing reduced Pc(3-) to Pc(5-) ligands and rare structurally characterized examples of these ring-reduced complexes with early transition-metals will be shown. Examples of applications of these new materials will be presented, including PcMn- and PcY-based systems in colour tuning, a mixed-sandwich PcU(COT) system for probing f-electron bonding, and PcZr-based materials as lactide polymerization catalysts.



Na(THF)PcZr(OiPr)$_3$ ate complex



Organometallic PcU(COT)

REFERENCES

Selected References: Y. Ganga-Sah, S. Holdcroft, D.B. Leznoff et al, *Chem Eur. J.*, **2025**, *31*, e02211; A. W./ Zhou, D. McKearney, G. Schreckenbach, D.B. Leznoff, *Inorg. Chem*., **2025**, *64*, 6857-6864; W. Zhou, D. McKearney, D.B. Leznoff, *Chem. Eur. J.*, **2020**, *26,* 1027-31; D. McKearney, M.S. Kim, N.E. Leznoff, C.C. Leznoff, D.B. Leznoff, *J. Porphyrins Phthalocyanines*, **2025**, *29*, 1231-1240; W. Zhou, D.B. Leznoff, *Chem. Commun.*, **2018**, *54*, 1829-1832; W. Zhou, N. Kobayashi, D.B. Leznoff et al, *Chem. Commun.,* **2025**, 3832-35; D. McKearney, D.B. Leznoff et al, *Chem. Commun.*, **2019**, *55*, 6696-6699; D. McKearney, D.B. Leznoff et al, *Dalton Trans.*, **2024**, *53*, 938-948.

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Porphyrin dyes for fabrication of highly efficient DSSCs: A concerted companion strategy

Chengjie Li[a], Conglin Liu[a], Yuquan Hu[a], Yinglong Li[a], Jiazhi Zou[a], Jiaxin Luo[a], Xueyan Wang[a], Yuqing Wang[a], Zhemin Li[a], Yingying Chen[a], Qingjun Lu[a], Kaiwen Zeng[a], Yongshu Xie[a]

[a]*Key Laboratory for Advanced Materials, School of Chemistry and Molecular Engineering, East China University of Science & Technology, Shanghai 200237, China.*

The use of solar energy is essential for reducing fossil fuel consumption and CO_2 emissions.[1] Among third-generation solar cells, dye-sensitized solar cells feature easy fabrication, low cost, reasonable power conversion efficiency, and colorful aesthetics, attracting considerable attention.[2] In DSSCs, the dyes play crucial roles by absorbing photons and pumping excited electrons into TiO_2. Till now, various dyes have been developed. As analogs of chlorophylls, porphyrins have been systematically optimized to develop high-performance dyes.[2] However, artificial porphyrin dyes feature weak absorption around 550 nm and in the near-infrared (NIR) region. To address this problem, intermolecular co-sensitization has achieved remarkable success by combining a porphyrin dye with one or more complementary-absorption dyes. For this strategy, time-consuming optimization of the bathing parameters (e.g., dye concentrations and sequential/cocktail/pre-adsorbing bathing methods) is necessary to achieve remarkable PCEs. As a complementary approach for intermolecular cosensitization, we have developed an intramolecular cosensation method to construct "concerted companion (CC)" dyes by covalently linking a porphyrin sub-dye with a spectral complementary organic dye.[3] Optimization of the linkage length, alkyl chain around the porphyrin framework, and the donor parts has been carried out to achieve the highest PCE up to 12.6%, based on the iodine electrolyte, under sunlight and 34.5% under dim light without using any co-adsorbent.[4-9]

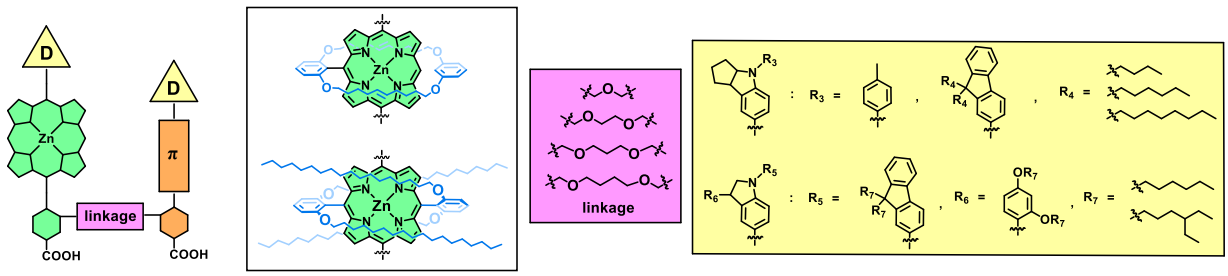


Figure 1. The common structure of CC-dyes and the optimization in different moieties.

REFERENCES

1. B. O'Regan and M. Grätzel, *Nature,* 353 (1991), 737-740.
2. K. Zeng, Z. Tong, L. Ma, et al., *Energy Environmental Science,* 13 (2020) 1617-1657.
3. K. Zeng, Y. Chen, W. Zhu, et al., *Journal of the American Chemical Society*, 142 (2020) 5154-5161.
4. J. Zou, Y. Wang, G. Baryshnikov, et al., *ACS Applied Materials & Interfaces,* 14 (2022) 33274-33284.
6. Z. Li, Q. Lu, Y. Zhang, et al., *Journal of Materials Chemistry A*, (2024) 4176-4185.
7. C. Liu, Y. Li, Y. Hu, et al., *Chinese Chemical Letters,* 37 (2026) 111863.
8. J. Luo, Y. Wang, S. Shi, et al., *Journal of Materials Chemistry C*, 11 (2023) 5450-5460.
9. X. Wang, Y. Wang, J. Zou, et al., *ChemSusChem*, 15 (2022) e202201116.

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Synthesis and properties of novel confused expanded porphyrinoids

Qizhao Li, Yongshu Xie

Key Lab for Advanced Materials, East China University of Science & Technology, Shanghai, China

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Porphyrin analogs (i.e., porphyrinoids) have attracted considerable attention due to their distinctive physicochemical properties that can be utilized for applications in various areas such as catalysis, photoacoustic dyes, nonlinear optical materials and photodynamic therapy[1]. In this regard, we have developed a series of novel confused expanded porphyrinoids via the "Confusion" approach involving the inclusion of α-β-linked pyrrole units into expanded porphyrins[2]. Thus, we have developed novel antiaromatic expanded porphyrins by oxidation of linear oligopyrrole with one terminal confused pyrrole unit[3]. The presence of reactive confused pyrrolic units endows these antiaromatic molecules with distinct chemical reactivities, enabling their readily transformation into novel aromatic and/or chiral macrocycles by further oxidation, reduction, coordination, acidification, etc[4-5]. Owing to the presence of the protruding N-confused pyrrole unit, some confused expanded porphyrins can undergo facile oxidative coupling dimerization, and the structures and properties of these molecules are further modulated and extended[6-9]. The resultant expanded porphyrin dimers show great potential for applications in small-molecule recognition, photodynamic therapy and photothermal therapy, highlighting the power of the confusion approach for developing novel macrocycles with unprecedented structures and functions.

REFERENCES

1. Tanaka, T.; Osuka, A. *Chem. Rev.* **2017**, *117*, 2584-2640.
2. Toganoh, M.; Furuta, H. *Chem. Rev.* **2022**, *122*, 8313-8437.
3. Li, Q.; Ishida, M.; Wang, Y.; Li, C.; Baryshnikov, G.; Zhu, B.; Sha, F.; Wu, X.; Ågren, H.; Furuta, H.; Xie, Y. *Angew. Chem. Int. Ed.* **2023**, *62*, e202212174
4. Li, Q.; Ishida, M.; Li, C.; Baryshnikov, G.; Sha, F.; Zhu, B.; Wu, X.; Ågren, H.; Furuta, H.; Xie, Y. *CCS Chem.* **2023**, *5*, 1332-1342
5. Li, Q.; Ishida, M.; Kai, H.; Gu, T.; Li, C.; Li, X.; Baryshnikov, G.; Liang, X.; Zhu, W.; Ågren, H.; Furuta, H.; Xie, Y. *Angew. Chem. Int. Ed.* **2019**, *58*, 5925-5929.
6. Li, Q.; Li, C.; Baryshnikov, G.; Ding, Y.; Zhao, C.; Gu, T.; Sha, F.; Liang, X.; Zhu, W.; Wu, X.; Ågren, H.; Sessler, J. L.; Xie, Y. *Nat. Commun.* **2020**, *11*, 5289.
7. Li, Q.; Li, C.; Kim, J.; Ishida, M.; Li, X.; Gu, T.; Liang, X.; Zhu, W.; Ågren, H.; Kim, D.; Furuta, H.; Xie, Y. *J. Am. Chem. Soc.* **2019**, *141*, 5294-5302.
8. Xie, Y.; Su, G.; Ishida, M.; Zhu, B.; Baryshnikov, G.; Sha, F.; Li, C.; Wu, X.; Ågren, H.; Furuta, H.; Li, Q. *J. Am. Chem. Soc.* **2025**, *147*, 5368-5376
9. Huang, Y.; Zhu, B.; Li, S.; Baryshnikov, G.; Wang, H.; Li, C.; Ågren, H.; Jiang, J.; Xie, Y.; Li, Q. *J. Am. Chem. Soc.* **2025**, *147*, 28161-28172.

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Bacteriochlorins and Porphyrin-Bacteriochlorin Dimers for Solar Cell Applications

Ching-Yao Lin, Hung-Ming Chang, Shao-Wei Hong, Ren-Bao Wu, Ming-Sin Liu, Chien-Lin Li, Sheng-Ting Wu, Hua-An Liu

Department of Applied Chemistry, National Chi Nan University, No. 302 University Road, Puli, Nantou Hsien 54561, Taiwan, R.O.C. Fax: +886-49-2917956; Tel: +886-49-2910960 ext. 4152; E-mail: cyl@ncnu.edu.tw

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Bacteriochlorins are vital to photosynthesis in bacteria. Nature occurring bacteriochlorins are, however, unstable without the protection of amino acids. For any applications, air-stable bacteriochlorins are, therefore, very important [1-3]. We herein report several air-stable, *meso*-substituted bacteriochlorins (denoted as the LS dyes). In addition to the monomeric bacteriochlorin dyes, we also investigated two porphyrin-bacteriochlorin dyes, denoted the LTD dyes. For fundamental properties, UV-visible absorption, fluorescent emission, electrochemistry, and DFT calculations are studied. For dye-sensitized solar cell applications, the photovoltaic performance of the LS- and LTD-cells is measured under one-sun irradiation.

REFERENCES

1. H.-J. Kim, J. S. Lindsey* *De Novo* Synthesis of Stable Tetra-hydroporphyrinic Macrocycles: Bacteriochlorins and a Tetradehydrocorrin. *J. Org. Chem.,* 2005*,* **70**, 5475-5486.
2. S. Chakraborty, H.-C. You, C.-K. Huang, B.-Z. Lin, C.-L. Wang, M.-C. Tsai, C.-L. Liu, C.-Y. Lin* *meso*-Diphenylbacteriochlorins: Macrocyclic Dyes with Rare Colors for Dye-Sensitized Solar Cells. *J. Phys. Chem. C,* 2017 *,* **121**, 7081 - 7087.
3. S. Chakraborty, M.-C. Tsai, X.-D. Su, X.-C. Chen, T.-T. Su, C.-K. Tsao, C.-Y. Lin* Synthesis, Properties and Photovoltaic Performance in Dye-Sensitized Solar Cells of Three *meso*-Diphenylbacteriochlorins Bearing a Dual-Function Electron-Donor, *RSC Adv.,* 2020*,* **10**, 6172-6178.

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Some results concerning tetrapyrrole synthesis methods

Duy T. M. Chung and Jonathan S. Lindsey

Department of Chemistry, North Carolina State University, Raleigh, NC 27695 USA

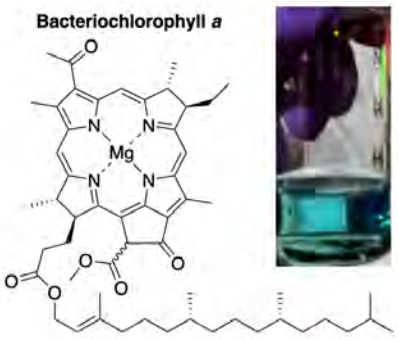
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New methods hold the promise of new vistas.

We recently completed the synthesis of bacteriochlorophyll *a* beginning with small molecules. Bacteriochlorophyll *a* contains the bacteriochlorin chromophore in the phorbin skeleton, 4 fixed stereocenters in the macrocycle, an epimerizable stereocenter embedded in the isocyclic ring, two stereocenters and an allylic alcohol in the phytyl unit, and is facially stereotopic as well.

Bacteriochlorophyll captivates us because (1) it is the key pigment of anoxygenic photosynthesis, and (2) it is among the most architecturally complex of photosynthetic tetrapyrroles. Points 1 and 2 comprise a conundrum if not a koan – how is it that the most complex pigment underpins the simplest photosynthetic system?

We are currently exploring the extension of the synthetic methodology developed for bacteriochlorophyll *a* to access a larger number of photosynthetic tetrapyrroles. The latter include the macrocycles, of which there are 15–20 of significance across photosynthetic systems, and the open-chain systems, namely the phyllobilins, of which there are >70 known to date. Native structures are obvious targets for proof of methodology; analogues are of interest for specific studies.



The presentation will survey the rationale for studying these neglected macrocycles [1] and some recent results from our lab in these regards.

This research is supported in part by the NSF (CHE-2348052).

REFERENCES

1. Total Synthesis Campaigns Toward Chlorophylls and Related Natural Hydroporphyrins – Diverse Macrocycles, Unrealized Opportunities. Liu, Y.; Zhang, S.; Lindsey, J. S. *Nat. Prod. Rep.* **2018**, *35*, 879–901.

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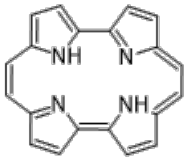
Porphycene and Corrphycene: Useful Objects for Intramolecular Hydrogen Bond Transfer Studies

Arkadiusz Listkowski,[a,b] Weronika Bodek,[b] Magdalena Piechocka,[b] Aleksandra Krogulska,[b] Michał Kijak,[a] and Jacek Waluk[a,b]

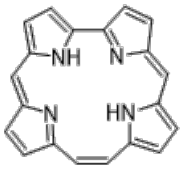
[a]*Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland*
[b]*Faculty of Mathematics and Natural Sciences, College of Science, Cardinal Stefan Wyszyński University, Dewajtis 5, 01-815 Warsaw, Poland*

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Porphycene, reported by Vogel in 1986,[1] is known as a first example of a porphyrin isomer. Owing to unique spectroscopic and photophysical properties, in addition to numerous potential applications typical of photoluminescent materials,[2] this compound is readily used in basic research, becoming, for example, an excellent model for studying the mechanism of intramolecular hydrogen transfer.[3] These possibilities also encouraged attempts to obtain further representatives of the porphyrinoid family. In 1994 the synthesis of *N*-confused porphyrin.[4,5] as well as corrphycene[6] were described. The latter compound, having all nitrogen atoms pointing towards the interior of the gap created by the pyrrole rings can serve as a model for similar studies as reported for porphycene. It is worth noting that corrphycene, unlike porphycene, belongs to the group of soft chromophores, in which the dependence of spectroscopic properties, such as electronic absorption or magnetic circular dichroism (MCD), on substituents is high.[7] The geometry of two hydrogen bonds present in both of this molecules can be easily modified by appropriate pattern of peripheral substituents, and asymmetric substitution leads to systems with non-equivalent hydrogen bonds, which can be observed and characterised by various spectroscopic methods. During the presentation, new methods of porphycene and corrphycene desymmetrization and its influence on the spectroscopic and photophysical properties of these compounds will be discussed.



Porphycene ("Hard")



Corrphycene ("Soft")

REFERENCES

1. E. Vogel, M. Kocher, H. Schmickler, J. Lex *Angew, Chem. Int. Ed. Engl.* **1986**, *25*, 257-259.
2. G. Anguera, D. Sanchez-García *Chem. Rev*. **2017**, *117*, 2481−2516
3. J. Waluk *Chem.Rev*. **2017**, *117*, 2447-2480
4. H. Furuta, T. Asano, T. Ogawa, *J. Am. Chem. Soc.* **1994**, *116*, 767-768.
5. P. J. Chmielewski, L. Latos-Grażyński, K. Rachlewicz, T. Głowiak, *Angew. Chem., Int. Ed. Engl.* **1994**, *33*, 779-781.
6. J. L. Sessler, E. A. Brucker, S. J. Weghorn, M. Kisters, M. Schäfer, J. Lex, E. Vogel *Angew. Chem. Int. Ed. Engl*. **1994**, *33*, 2308-2312.
7. A. Listkowski, M. Piechocka, M. Kijak, R. Rybakiewicz-Sekita, R. Luboradzki, J. Waluk *Chem. Eur. J*. **2025**, **31**, e202500779.

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Quantum Dynamics of Hydrogen Transfer in Porphycene: From Gas Phase to Adsorption on Metal Surfaces

Yair Litman[a]

[a]*Max Planck Institute for Polymer Research, Mainz, Germany*

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Hydrogen transfer in molecular systems challenges our understanding of chemical reactivity, especially when nuclear quantum effects (NQEs) such as tunneling and zero-point motion play a dominant role. Porphycene, a prototypical system with strong intramolecular hydrogen bonds and complex double-hydrogen-transfer (DHT) dynamics, offers a rich playground for exploring these effects across different environments and observables. In this talk, I will present a unified perspective on hydrogen dynamics in porphycene, going from the gas phase to its adsorption on metal surfaces.

Using state-of-the-art path-integral methods combined with first-principles electronic structure theory and machine learning approaches, we studied the hydrogen-transfer mechanisms, tunneling rates, and vibrational spectroscopy of porphycene [1,2,3]. Our findings consistently show that strong anharmonic coupling between low- and high-frequency modes leads to a complex quantum behavior. In the gas phase, this manifests as a strong temperature dependence of the hydrogen tunneling rates and unconventional features in the vibrational spectra. Upon adsorption on metallic surfaces, coupling to surface-induced fluctuations dramatically reshapes the tunneling landscape, enhancing reaction rates even in the deep-tunneling regime. Together, these results provide a comprehensive picture of hydrogen dynamics in complex molecular systems and highlight the decisive role of NQEs, anharmonicity, and multidimensional vibrational mode coupling.

REFERENCES

1. Y. Litman, J. O. Richardson, T. Kumagai, M. Rossi, J. Am. Chem. Soc. **141**, 6, 2526–2534 (2019)
2. Y. Litman, J. Behler, Mariana Rossi, Faraday Discuss., **221**, 526-546 (2020)
3. Y. Litman, M. Rossi. Phys. Rev. Lett. **125**, 216001 (2020)

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Synthesis of Neo-triphyrin(0.1.1)

Runchang Liu[a], **David Dolphin**[b]

[a]*ATA Law Corporation (Canada)*
[b]*University of British Columbia*

In 2011, Furuta and co-workers reported the identification of a nitrogen–carbon–linked tetraporphyrinoid structure, termed norrole,[1] which was synthesized through a multistep procedure. Around the same time, Lash and his colleagues reported a porphyrin isomer, known as neo-confused porphyrin, by employing an *N*–meso–*C* connected dipyrrolemethane as the key building block.[2] Meanwhile the synthesis of the presently reported N–C–linked neo-triphyrin was also independently achieved in our laboratory in 2011.

We report here the first synthesis and structural characterization of Neo-triphyrin(0.1.1), the smallest N–C bond linked porphyrinoid macrocycle. The 12π tripyrrolic system, obtained via a one-pot condensation and DDQ oxidation, features two N-confused pyrroles connected through direct N–C linkages. X-ray diffraction confirmed a planar tripyrrolic structure stabilized by intramolecular C=O···π and hydrogen-bonding interactions. This work establishes a new design principle for N–C bond cyclization in porphyrinoid chemistry.

As the smallest N-confused porphyrinoid macrocycle reported to date, neo-triphyrin(0.1.1), featuring a 12π antiaromatic system, was fully characterized. Its molecular structure was unambiguously established by single-crystal X-ray diffraction. The macrocycle exhibits distinctive structural features arising from its N-confused framework. Its antiaromatic character is further supported by nucleus-independent chemical shift (NICS) calculations performed using Gaussian. Importantly, the directing synthetic strategy employed herein provides a rational and potentially generalizable platform for controlling pyrrole inversion and stabilizing N-confused topologies, thereby enabling the targeted discovery and isolation of previously inaccessible NCP-type macrocycles.

REFERENCES

1 Fujino, K.; Hirata, Y.; Kawabe, Y.; Morimoto, T.; Srinivasan, A.; Toganoh, M.; Miseki, Y.; Kudo, A.; Furuta, H. *Confusion and Neo Confusion: Corrole Isomers with an NNNC Core.* **Angew. Chem., Int. Ed. 2011**, *50* (30), 6855–6859.
2 Lash, T. D.; Lammer, A. D.; Ferrence, G. M. Neo Confused Porphyrins, *a New Class of Porphyrin Isomers.* ***Angew. Chem.,*** **Int. Ed. Engl. 2011**, 50 (41), 9718–9721.

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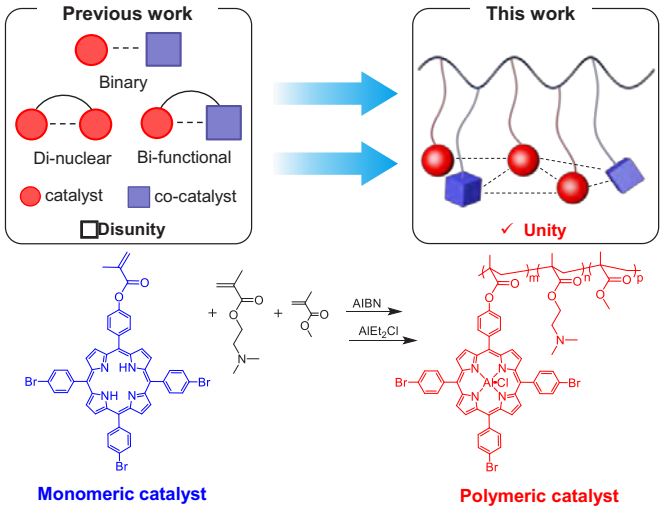
Efficient Synthesis of CO_2-Polyols by Polymeric Aluminum Porphyrin Catalysts

Shunjie Liu[a,b], **Xianhong Wang**[a,b]

[a]*State Key Laboratory of Polymer Science and Technology, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences; No.5625, Renmin Street, Changchun, Jilin, 130022, P. R. China*
[b]*School of Applied Chemistry and Engineering, University of Science and Technology of China; No.96, JinZhai Road, Hefei, Anhui, 230026, P. R. China*
E-mail: sjliu@ciac.ac.cn, xhwang@ciac.ac.cn

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Carbon dioxide-based polymer polyols (CO_2-polyol) are emerging as promising polyurethane precursors due to their economic and environmental advantages. However, the sustainable development of this field is hindered by the limited availability of efficient catalytic systems, primarily because most current catalysts exhibit poor proton tolerance. In this report, we propose a strategy to construct polymeric catalysts by incorporating active centers into a single polymer chain.[1,2] Unlike conventional single-site catalysts, which lose activity under dilute conditions, the resulting polymeric aluminum porphyrin catalysts—featuring multiple aluminum porphyrin complexes anchored on the side chains—demonstrate excellent polyols selectivity (>99%) and high polymerization rate (turnover number > 50,000). Furthermore, this approach enables the production of colorless CO_2-polyol with an ultralow molecular weight (<500 g/mol), thanks to the enhanced proton tolerance.



REFERENCES

1. H. Cao, Y. Qin, C. Zhuo, X. Wang, F. Wang, ACS Catal. 2019, 9, 8669-8676.
2. Q. Kuang, R. Zhang, Z. Zhou, C. Liao, S. Liu, X. Chen, X. Wang, Angew. Chem. Int. Ed. 2023, e202305186.

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Development of Novel Photosensitizers for Inducing Immunogenic Cell Death in Photodynamic Therapy

Pui-Chi Lo, Feijie Xu, Yuanfeng Zhang, Kwan T. Chow, Meijun Wang

Department of Biomedical Sciences, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong, China

Photodynamic therapy (PDT) is an innovative treatment modality that harnesses the power of light-activated photosensitizers to selectively target and destroy cancer cells. This approach involves administering a photosensitizing agent that preferentially accumulates in tumor tissue. Upon exposure to specific wavelengths of light, the photosensitizer is activated, generating reactive oxygen species (ROS). These ROS induce cellular damage, resulting in non-immunogenic or immunogenic cell death pathways. The immunogenic nature of cell death induced by PDT is more favorable as it can stimulate systemic anti-tumor immune responses, thereby enhancing overall therapeutic efficacy [1]. Despite its potential, PDT's effectiveness can be limited by factors such as the hypoxic tumor microenvironment and antioxidant defenses. Therefore, the development of novel photosensitizers capable of overcoming these challenges and inducing immunogenic cell death is critical. This study focuses on the design and synthesis of photosensitizers that target disease-related proteins, such as glutathione peroxidase 4 (GPX4) and cyclooxygenase-2 (COX-2), to trigger immunogenic cell death via ferroptosis and pyroptosis, thereby enhancing photoimmunotherapy [2-3]. We found that photosensitization of GPX4 by PDT could induce lipid peroxidation and oxidative stress, triggering ferroptosis, while PDT-induced COX-2 suppression could reduce prostaglandin E2 synthesis, converting the immunosuppressive microenvironment into an immunostimulatory one. These hypotheses are validated through a series of in vitro experiments using various cell lines and in vivo mouse xenografts.

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REFERENCES

1. Alzeibak, R.; Mishchenko, T. A.; Shilyagina, N. Y.; Balalaeva, I. V.; Vedunova, M. V; Krysko, D. V. Targeting immunogenic cancer cell death by photodynamic therapy: past, present and future. *J. Immunother. Cancer* 2021, 9, e001926.
2. Zhang, Y.; Wang, M.; Chow, K. T.; Lo, P.-C. Unpublished results.
3. Xu, F.; Wang, M.; Chow, K. T.; Lo, P.-C. Unpublished results.

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Designing biosynthetic models of heme-copper enzymes to understand oxidase and sulfite reductase catalysis

Yi Lu,* Yiwei Liu, Aaron P. Ledray, and Barshali Ghosh

Department of Chemistry, The University of Texas at Austin

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Heme-copper oxidases (HCOs) are terminal oxidases that catalyze the oxygen reduction reaction (ORR), providing energy for ATP synthesis that sustains most biological processes. While a His-Tyr crosslink is proposed to be essential for HCO's oxidase activity, its formation mechanism and the specific functional roles remained elusive since its discovery over 30 years ago. A major barrier is the inability to isolate HCO prior to the crosslink formation, which precludes direct comparisons with its crosslinked form. To address this issue, we designed a biosynthetic model of HCO using sperm whale myoglobin (swMb), which exhibited ORR activity comparable to that of native HCO. We discovered a novel His-His crosslink and a Tyr-His crosslink in the model of F33Y-Cu_BMb, together with the characterization, formation mechanism and resulting impact on ORR activity [1]. A mechanistic study also revealed a compound II ferryl species and the Tyr33 radical, which together lead to crosslink formation. Notably, upon formation of the His29-His43 crosslink, F33Y-CuBMb displayed nearly tripled four-electron ORR activity at pH 7.0 and partially retained up to pH 9.5, whereas the pre-crosslinked F33Y-Cu_BMb became inactivated above pH 8.0. Based on these results, we propose a self-processing mechanism for crosslink formation, including Tyr-His and His-His. Through the discovery of the enzymatically unprecedented His-His crosslink in a biosynthetic model, this study contributes to understanding the formation mechanism of active site crosslinks in natural oxidoreductases and presents a facile but unexplored approach to fine-tuning enzymatic activity. Building upon these findings, we have further improved the models to allow a His-Tyr cross-link like in native HCOs.

Interestingly, both HCO and sulfite reductase type A (SiR-A) rely on a copper center next to heme to perform their biological reactions, but a question remains as to why the Cu_B center in HCO promotes ORR that is essential for generating a proton motive force to synthesize ATP in aerobic life, while the Cu_{SiR} in SiR-A is efficient at sulfite reduction reaction (SRR) to sulfide to generate a proton motive force in anaerobic bacteria. To answer this question, we designed either a Cu_B or a Cu_{SiR} within a single protein scaffold, soybean ascorbate peroxidase (APX), to mimic those in HCO and SiR-A, respectively [2]. By eliminating confounding factors from different native scaffolds, our approach isolates the intrinsic roles of copper coordination environments in dictating catalytic specificity. This unique strategy offers unprecedented clarity on how these centers govern oxygen and sulfite reduction. Our results show that, while both Cu_B and Cu_{SiR} can catalyze ORR, only CuSiR can perform SRR. This difference in the cross reactivity indicates that it may be easier to perform ORR that requires 4e and $4H^+$ than SRR that requires 6e and $7H^+$. Interestingly, while introducing a Tyr in Cu_BAPX increased ORR activity, a surprising finding is that the same variant also increased SRR, resulting in the total activity that is even higher than that of Cu_{SiR}APX. These findings underscore the role of the Cu-ligating residues shaping enzyme specificity for oxygen versus sulfite reduction and highlight how nature has evolved distinct heme-Cu motifs in conjunction with redox-active residues to meet the demands of aerobic and anaerobic lives.

REFERENCES

1. Yiwei Liu, Avery C. Vilbert, Barshali Ghosh, Robert P. Young, Eric D. Merkley, Arnab Mukherjee, Lisa Phan, Casey Van Stappen, Ambika Baghi-Damodaran, Kyle D. Miner, Joshua Adkins, John Cort, and Yi Lu, *J. Am. Chem. Soc.* 2025, 147, 41, 37688–37700 (2025)
2. Aaron P. Ledray, Barshali Ghosh, Hirbod Heidari, Yi Lu, manuscript under review

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Phthalocyanine-based Edible Electronics

Alessandro Luzio, Mario Caironi

Center for Nano Science and Technology (CNST), Istituto Italiano di Tecnologia (IIT), Via Raffaele Rubattino 81, 20134, Milano, Italy

Edible Electronics aims to develop fully edible electronic systems for applications ranging from gastrointestinal monitoring to food-quality assessment and transient biointerfaces [1]. A key challenge is identifying safe semiconductors that enable active, low-power electronic components to safely transit the gastrointestinal tract. In response to this need, this talk presents an overview of phthalocyanine-based edible electronics, highlighting the key concepts, materials, and device strategies underpinning this approach.

This work is grounded in the validation of phthalocyanine pigments as safe and effective semiconductor ingredients. These pigments are among the most widely used commercial colorants due to their chemical stability, high tinting strength, and low toxicity. Beyond their semiconducting properties, their routine use as colorants and whitening additives in commercial toothpastes provides direct evidence of their safety for ingestion in quantities far exceeding those required in our devices 2]. The talk then illustrates how microstructural control and solution-based processing routes yield high-performance electrical films through fabrication methods suitable for fully edible system integration, and how these approaches enable the upcycling of colorant-grade phthalocyanines into functional semiconductor materials [3]. Building on this framework, fully edible phthalocyanine-based active components are finally presented, including logic gates, platforms for chemical and physiological monitoring, in situ signal generation, and neuromorphic devices.

These results position phthalocyanine-based electronics as a versatile foundation for future edible sensing, logic, neuromorphic, and bio-interfacing technologies.

REFERENCES

1. A. Sharova, F. Melloni, G. Lanzani, C. J. Bettinger, M. Caironi, Adv. Mat. Technol. “Edible electronics: The vision and the challenge”, 6(2), 2000757 [1] A. Sharova, F. Melloni, G. Lanzani, C. J. Bettinger, M. Caironi, Adv. Mat. Technol. “Edible electronics: The vision and the challenge”, 6(2), 2000757
2. E. Feltri, P. Mondelli, B. Petrović, F. M. Ferrarese, A. Sharova, G. Stojanović, A. Luzio, M. Caironi, A Fully Edible Transistor Based on a Toothpaste Pigment. Adv. Sci. 2024, 11, 2404658. https://doi.org/10.1002/advs.202404658
3. A. Luzio, F. M. Ferrarese, M. Butti, A. D. Scaccabarozzi, B. Petrović, S. Kojić, G. Stojanović, S. Fiorini Granieri, S. Tanwar, A. Kyndiah, M. Caironi, A Solution-Based Deposition Method Enabling Pigment Blue Edible Electrochemical Transistors. Adv. Sci. 2025, 12, 2416141. https://doi.org/10.1002/advs.202416141

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Design and Application of Porous Porphyrin-Derivative Frameworks

Shengqian Ma

Department of Chemistry. University of North Texas. USA.

Over the past two decades, rapid growth has been observed in the fields of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs), which feature tunable, designable, and functionalizable nanospace. The utilization of new types of organic ligands for the construction of MOFs/COFs has long been sought after, as evidenced by the success in porphyrin-based MOFs/COFs. Beyond porphyrins, we show that their derivatives, corroles and rosarins, can be employed as new building blocks to construct porous framework materials with interesting properties in catalysis and electronics.

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Charged Zinc Phthalocyanines – are they suitable for PDT, VTP, PCI or PDI?

Miloslav Macháček[a], Ingrid Hlbočanová[a], Pavlína Vávrová[b], Khaoula Lmcharrag[c], Klára Konečná[b], Magdaléna Kozlíková[a], Monika Rohlíčková[a], Veronika Nováková[c] and Petr Zimčík[c]

[a] *Department of Biochemical Sciences,* [b] *Department of Biological and Medical Sciences,* [c] *Department of Pharmaceutical Chemistry and Pharmaceutical Analysis, Faculty of Pharmacy in Hradec Králové, Charles University, Czech Republic; machamil@faf.cuni.cz*

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Phthalocyanines (Pcs) are well-known and highly effective photosensitizers (PSs) that have proven suitable for a wide range of biomedical applications – photodynamic therapy (PDT), vascular-targeted PDT (VTP), photochemical internalization (PCI), photodynamic inactivation of microorganisms (PDI), and more. Structural modifications of the Pc core yield a myriad of compounds with distinct properties (e.g., variations in symmetry, central metal ions or substituents). While the unsubstituted Pc core is a planar and highly lipophilic structure prone to aggregation and therefore poorly suited for aqueous environments, appropriate structural modifications can effectively overcome this poor solubility in water-based media. On the other hand, are the highly hydrophilic non-aggregating Pc-based PSs the best candidates in all biomedical applications?

Cell-based assays (on 2D models) showed clear relationships between charge (cationic vs. anionic), symmetricity (symmetrical hydrophilic vs. unsymmetrical amphiphilic), and photodynamic activity [1]. These trends were, to some extent, confirmed on 3D models and an *in vivo* mouse tumor model (PDT and VTP): symmetrical cationic derivatives were more potent than unsymmetrical derivatives (both anionic and cationic), while symmetrical anionic ones exhibited the lowest activity. Unsymmetrical PSs are particularly effective in PCI, and out our derivatives demonstrate the same advantage, successfully mediating intracellular delivery of model cargo uch as saporin or gelonin.

Abovementioned treatment modalities are usually used against cancer. But what about directing PDT effect against microorganisms (MOs) through PDI? In our study we focused on pathogens represented by the acronym ESKAPE: gram-positive bacteria (methicillin resistant *Staphylococcus aureus* (MRSA), *Enterococcus faecium*) and gram-negative bacteria (*Pseudomonas aeruginosa*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Enterobacter cloaceae*). All MOs were incubated with PSs for 30 min, washed and subsequently irradiated with Xe lamp (λ > 570 nm, 15 min, 11.2 J/cm^2). Growth curves were measured for 24 h using Bioscreen C. As a reference PSs, we used methylene blue, new methylene blue, toulidine blue O, and rose bengal. In addition, cytotoxicity toward normal human cells was evaluated using fibroblasts (MRC-5), endothelial cells (HUVECs) and keratinocytes (HaCaT). Human skin permeation was assessed using Franz diffusion cells, and localization within human skin was examined using confocal microscopy. The amphiphilic cationic derivative exhibited superior antimicrobial activity, achieving an MBC of 100 nM and inducing 3-log reduction at 5 nM (MRSA), whereas the hydrophilic anionic Pc failed to reach a 3-log reduction even at highest dose evaluated (200 µM).

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REFERENCES

1. Kollar J; Machacek M; Halaskova M; Lenco J; Kucera R; Demuth J; Stekla M; Hasonova K; Miletin M; Novakova V; Zimcik P. *Journal of Medicinal Chemistry*. **2020**; 63(14); 7616-7632

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Meso-group Functionalization and Nanoparticle Conjugation of Porphyrinoid Singlet Oxygen Photosensitizer Dyes for Biomedical Applications

John Mack, Rodah Soy, Gugu Kubheka, Nthabeleng Molupe, Godfred Sebiawu, Mahlatse Ledwaba, Temlandvo Magwaza, Kaisano Tauyakhale, Vicky Laure Kembou, Pertunia Macigane, Zine Gwaji, Liyema Makeleni, Shakhola Sekeleme, Nolwazi Zitha, Tebello Nyokong

Tebello Nyokong Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa

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Over the last seven years, considerable progress has been made with a rational structural modification approach [1,2] guided by an application of Michl's perimeter model to prepare porphyrin analogues with significantly red-shifted and intensified Q bands that are suitable for use as photosensitizer dyes in photodynamic therapy (PDT) and/or photodynamic antimicrobial chemotherapy (PACT) [2,3]. When corroles, chlorins and N-confused porphyrins are formed by introducing a pyrrole-pyrrole bond, a reduced peripheral pyrrole bond and a confused pyrrole nitrogen atom, respectively, there is a significant red shift of the lowest energy Q band into the therapeutic window (620−850 nm) relative to the parent metal porphyrin and singlet oxygen quantum yields can be enhanced through coordination of a heavy central atom [2]. Significant absorption in the 700−800 nm region and relatively high singlet oxygen quantum yields can also be achieved through the halogenation of π-extended BODIPYs [4] and azaBODIPY dyes [5]. The introduction of thienyl or methylthiophenyl rings as *meso*-substituents to tetraarylporphyrins [6] and triarylcorroles [3,7] or as proximal or distal substituents to 1,3,5,7-tetraarylazaBODIPY dyes [5,8] facilitates the preparation of gold and silver nanoparticle conjugates and significantly enhances the PDT and/or PACT activities of the dyes. Significantly lower IC_{50} values have been obtained for the gold and silver nanoparticle conjugates during *in vitro* photocytotoxicity studies against breast cancer cells relative to the parent photosensitizer dyes, and high log reduction values have been observed against both planktonic and biofilm cells of Gram-(+) *S. aureus* and Gram-(−) *E. coli* bacterial strains. Peripheral substitution of peripheral aryl rings has also been used to enhance the cell and mitochondria-targeting properties of the photosensitizer dyes [9] and to enhance their utility for photoelectrochemical sensing applications [10]. Further progress made in studies that are currently underway in this regard, and also on the PDT and PACT activities of the gold and silver nanoparticle conjugates of other porphyrin analogues, will be described.

REFERENCES

1. Mack J, *Chem. Rev.* 2017; **117**: 3444-3478.
2. Babu B, Mack J, Nyokong T, *Dalton Trans.* 2023; **52**: 5000-5018
3. Soy RC, Babu B, Mack J, Nyokong T, *Dyes Pigments* 2021; **194**: 109631.
4. Kubheka G, Babu B, Prinsloo E, Kobayashi N, Mack J, Nyokong T, *J. Porphyrins Phthalocyanines* 2021; **25**: 47-55.
5. Magwaza TM, Molupe N, Openda YI, Mack J, Nyokong T. *Photodiagn. Photodyn. Ther.* 2025; **55**: 104781.
6. Soy RC, Mafukidze D, Mack J, Nyokong T. *Eur. J. Inorg. Chem.* 2024; **27**: e202400072.
7. Soy RC, Macigane P, Mack J, Nyokong T, *J. Porphyrins Phthalocyanines* 2024; **28**: 469-486.
8. Kubheka G, Magwaza T, Mack J, Nyokong T, Shen Z, *J. Porphyrins Phthalocyanines* 2025; **29**: 71-83.
9. Babu B, Mack J, Nyokong T, *New J. Chem.* 2022, **46**, 5288-5295.
10. Shanmugam ST, Trashin S, De Wael K, *Biosens. Bioelectron.* 2022; **195**: 113652.

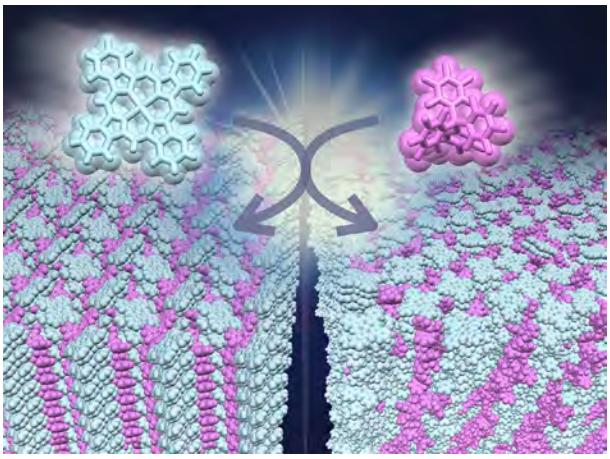
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Porphyrin-based ion-pairing assembly

Hiromitsu Maeda

Department of Applied Chemistry, College of Life Sciences, Ritsumeikan University, Kusatsu, 525–8577, Japan, maedahir@ph.ritsumei.ac.jp



Charged π-electronic systems with appropriate geometries and peripheral substituents provide assemblies through the interactions between charged building subunits, resulting in fascinating electronic properties [1]. Structures and properties of the assemblies can be controlled by the combined positively and negatively charged species in the assemblies [2,3]. π-Electronic ion pairs, including those of porphyrin-based cations and anions, have exhibited characteristic assembly modes via ${}^{i}\pi$–${}^{j}\pi$ interactions that are mainly ascribable to electrostatic and dispersion forces. The porphyrin anions with porphyrin–Au^{III} complexes as π-electronic cations provided various ion pairs in the form of π-stacked ion pairs (*π-sips*), whereas the "activated" porphyrin ion pair according to the *meso*-aryl substituents produced the π-stacked radical pair (*π-srp*) via the electron transfer in the ground state [2b]. Further design and modifications of charged porphyrins have been examined for the assemblies and electronic properties that are derived from ion pairing [2c–e]. As an example, the ion pair of an amphiphilic porphyrin Au^{III} complex bearing hydrophilic TEG-substituted aryl groups with a π-electronic anion formed charge-by-charge-based thermotropic and lyotropic liquid crystals and single-stranded polymer structure via amphiphilic ${}^{i}\pi$–${}^{j}\pi$ interactions [2c]. The positions and numbers of hydrophilic aryl groups control the assembly modes as seen in lamello-columnar (Lam_{col}) phases via amphiphilic ${}^{i}\pi$–${}^{j}\pi$ interactions for the charge-by-charge columns and lateral hydrophobic effects at the unsubstituted sites [2e]. Furthermore, the ion pairs of benzoporphyrin Au^{III} complex, with an extended charged π-system, formed charge-segregated assemblies as two pseudo-polymorphs of single-crystal and less-crystalline (LeC) states based on the stacking of the cations [2d].

REFERENCES

1. Reviews: (a) Haketa, Y.; Yamasumi, K. et al. *Chem. Soc. Rev.* **2023**, *52*, 7170. (b) Haketa, Y. et al. *Responsive Mater.* **2023**, *1*, e20230018. (c) Horita, H. et al. *Chem. Asian J.* **2025**, *20*, e70454.
2. (a) Sasano, Y.; Tanaka, H. et al. *Chem. Sci.* **2021**, *12*, 9645. (b) Tanaka, H. et al. *J. Am. Chem. Soc.* **2022**, *144*, 21710. (c) Maruyama, Y. et al. *Angew. Chem. Int. Ed.* **2025**, *64*, e202415135. (d) Haketa, Y.; Nakajima, R. et al. *Chem. Sci.* **2025**, *16*, 4998. (e) Maruyama, Y. et al. *Small* **2026**, *22*, e11729.
3. (a) Yamasumi, K. et al. *Angew. Chem. Int. Ed.* **2023**, *62*, e202216013. (b) Sugiura, S. et al. *J. Am. Chem. Soc.* **2023**, *144*, 8122. (c) Haketa, Y.; Komatsu, K. et al. *Chem. Sci.* **2024**, *15*, 964. (d) Yamasumi, K.; Horita, H. et al. *Chem. Eur. J.* **2025**, *31*, e202404781. (e) Kitayama, R. et al. *Chem. Eur. J.* **2025**, *31*, e02225. (f) Kobayashi, H. et al. *Chem. Eur. J.* **2025**, *31*, e02698.

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Electropolymerized Phthalocyanines and Corroles: Tunable Porphyrinoid Polymers for Chemical Sensing

Gabriele Magna[a], Mélanie Cyr[b,c], Francesco Pizzoli[a], Jaclyn L. Brusso[b], Benoît H. Lessard[c], Corrado Di Natale[d], Roberto Paolesse[a]

[a]*Department of Chemical Sciences and Technology, Tor Vergata University of Rome, Rome, Italy*
[b]*Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa, Canada*
[c]*Department of Chemical and Biological Engineering, University of Ottawa, Ottawa, Canada*
[d]*Department of Electronic Engineering, Tor Vergata University of Rome, Rome, Italy*

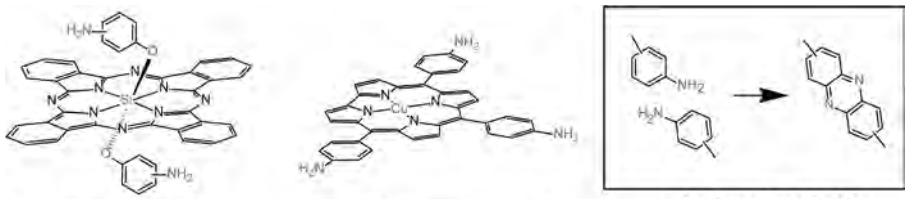
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Porphyrinoid-based materials offer a unique combination of extended π-conjugation, redox activity, and structural modularity, making them highly attractive for the design of functional organic conductors and sensing polymers [1]. In this work, we investigate electropolymerized porphyrinoid systems derived from structurally distinct macrocycles, namely axially functionalized silicon phthalocyanines and peripherally substituted copper corroles, as active materials for chemical sensing applications .

Novel para-, meta-, and ortho-bis(aminophenoxy) silicon phthalocyanines were selected as model systems to explore axial polymerization pathways enabled by the silicon center, which allows polymer growth without direct involvement of the phthalocyanine π-system. This structural feature promotes the formation of polymeric networks in which the phthalocyanine cores act as electronically active, spatially separated recognition units. In contrast, a 5,10,15-tris(4-aminophenyl)copper corrole was employed to achieve peripheral polymerization, generating conductive films in which the macrocyclic framework directly participates in charge transport while preserving accessibility to the metal center. Electropolymerization was carried out using cyclic voltammetry and chronoamperometry, providing complementary control over film growth, thickness, and morphology. The resulting films were integrated onto piezoelectric quartz microbalances (QMBs) and interdigitated electrodes (IDEs), where analyte adsorption induces either measurable frequency shifts or changes in film conductivity.

The sensing response of the porphyrinoid polymer films was evaluated toward gases, volatile organic compounds, and humidity. While individual materials exhibit broad and partially overlapping sensitivities, their responses strongly depend on both molecular structure, morphology, polymerization method, and transduction mechanism.

Overall, this study demonstrates how the interplay between porphyrinoid molecular design, polymerization strategy, and transduction mechanism can be harnessed to engineer tunable sensing materials. Electropolymerized silicon phthalocyanines and corroles emerge as a versatile and underexplored class of conductive polymers, well-suited for integration into multi-parameter sensing and electronic-nose architectures.



REFERENCES

1. Day, N.U., Walter, M.G., Wamser, C.C., *The Journal of Physical Chemistry C*, **2025**, *119*(30), 17378-17388.
2. Di Zazzo, L., et al. *Advanced Sensor Research,* **2024***,* 3(10), 2400005.

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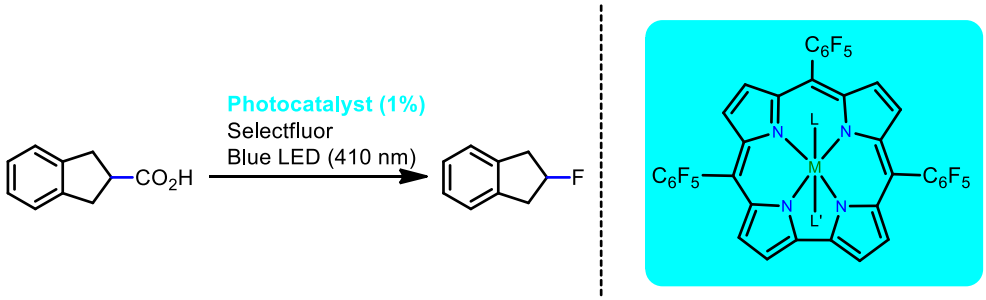


Metallocorroles as High-Performance Photoredox Catalysts for Decarboxylative Fluorination

Atif Mahammed, Qiu-Cheng Chen, and Zeev Gross*

Technion- Israel Institute of Technology, Schulich Faculty of Chemistry, Haifa 32000, Israel. Email: chatif@technion.ac.il, chr10zg@technion.ac.il

The expansion of photoredox catalysis into fields such as biology and materials science requires robust chromophores that operate efficiently under diverse conditions. Metallocorroles have recently emerged as powerful triplet photosensitizers and electrocatalysts owing to their tunability of redox potentials and optical excitation energies.[1-3] Here we demonstrate the photoredox activity of a broad family of corrole complexes in decarboxylative fluorination reactions. Phosphorus and antimony corrole complexes exhibit exceptionally long triplet lifetimes, which correlate strongly with their superior catalytic performance relative to $Ru(bpy)_3^{2+}$, enabling ~100-fold higher turnover frequencies with lower catalyst loadings. Mechanistic studies, including isolation of a highly reactive intermediate, clarify the catalytic cycle. Furthermore, these complexes efficiently promote the decarboxylative fluorination of common drug-related contaminants under mild yellow-light irradiation. These results position metallocorroles as promising and tunable platforms for next-generation photoredox transformations.



REFERENCES

1. A. Mahammed, H. B. Gray, Z. Gross, "Silver Anniversary of the Renaissance in Metallocorrole Chemistry" *Chem. Rev.* **2025**, *124*, 2809-2845.
2. T. Ianovici, W. Sinha, V. K. Sharma, S. Manna, D. Samanta, A. Mahammed, S. P. Rath, Z. Gross "Green Light for Photoredox Catalysis by Corroles and Porphyrins" *J. Porphyrins Phthalocyanines* **2025**, *29*, 751-758.
3. A. Mahammed and Z. Gross "Corroles as Triplet Photosensitizers" *Coord. Chem. Rev.* **2019**, *379*, 121-132.

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Peptide- and DNA-based heme protein models – spectroscopic insight

Piotr J. Mak[a]

[a]*Saint Louis University, Department of Chemistry, Saint Louis, MO 63103, USA*

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Iron(III) protoporphyrin IX (heme *b*) is a key cofactor involved in metabolic, catabolic, and cellular sensing processes. In natural heme proteins, the surrounding protein scaffold modulates the intrinsic reactivity of the heme group, enabling specific functions—such as peroxidase, oxygenase, or peroxygenase activity—while suppressing others. Although native heme proteins are highly effective catalysts, they are prone to degradation and sensitive to environmental conditions, limiting their stability and utility in industrial or therapeutic contexts.

Artificial metalloenzymes, including de novo heme-binding proteins, offer a controlled platform for probing the primary and secondary coordination spheres that govern heme reactivity. Such systems can be systematically engineered to achieve catalytic profiles that match or exceed those of natural proteins. We report spectroscopic studies of artificial heme-containing scaffolds capable of exhibiting both peroxidase-like activity and oxygenase reactivity.[1,2] Resonance Raman spectroscopy enables precise monitoring of pH dependent changes in heme ligation, revealing a shift between imidazole and thiolate bound states and providing insight into proximal ligand preferences.

Similarly, certain heme bound guanine quadruplexes (heme G4) display enhanced peroxidase activity and hold promise as DNA-based biocatalysts.[3,4] Despite extensive investigation, the mode of heme coordination in these DNA scaffolds remained speculative. Our spectroscopic data provide clear evidence that the guanine oxygen atom serves as an axial ligand, supported by the identification of an isotopically sensitive $\nu(Fe–O_G)$ stretching mode at 563 cm^{-1} in ferric heme G4 complexes.[5] These findings offer structural insights into the mechanisms driving the elevated peroxidase activity of heme G4 systems and inform the design of improved nucleic-acid-based biocatalysts.

REFERENCES

1. Koebke, K. J.; Kühl, T.; Lojou, E.; Demeler, B.; Schoepp-Cothenet, B.; Iranzo, O.; Pecoraro, V. L.; Ivancich. A. *Angew. Chem. Int. Ed.* **2021**, *60*, 3974-3978.
2. Modenez, I. A.; Ivancich, A.; Pecoraro. V. L. *Methods Enzymol*. **2025**, 720, 115-139.
3. Travascio, P.; Li, Y.; Sen, D. *Chemistry & biology* **1998**, *5*, 505-517.
4. Zhang, M.; Xu, S.; Minteer, S. D.; Baum, D. A. *J. Am. Chem. Soc.* **2011**, *133*, 15890-15893.
5. Chiura, T.; Pham, M.; Baum, D. A.; Mak, P. J. *J. Inorg. Biochem.* **2025**, *266*, 112843.

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Rational Design of Light-Induced Disruptive Porphysomes for Improved Photodynamic Therapy Applications

Khatia Merabishvili [a], Isokjon Pozilov [a], Jana Alhoussein[a], Christophe Regeard[b], Ali MAKKY[a]

[a] *Université Paris-Saclay, CNRS, Institut Galien Paris-Saclay, Bâtiment Henri Moissan, 17, Avenue des Sciences, 91400, Orsay, France*
[b] *Université Paris-Saclay, CEA, CNRS, Institute for Integrative Biology of the Cell (I2BC), 91198, Gif-sur-Yvette, France*

Porphyrins derivatives are naturally occurring macrocyclic molecules known for their efficiency in PDT applications when they are in their monomeric form.[1] However, the hydrophobic nature of porphyrins leads to their aggregation in biological environments thus reducing their efficiency and complicating administration. To overcome these drawbacks, several strategies have been tested either in preclinical studies or in clinical applications. This includes the usage of co-solvents (e.g. ethylene glycol, propylene glycol), the incorporation into liposome bilayers (Visudyne ®, Foslip and Fospeg) or even the complexation with polymers (Photolon®). While these strategies enhance solubility and delivery, they often fail to support high concentrations of porphyrin derivatives, which limits the potency, and therapeutic extent of PDT.

Herein, we present the design of smart supramolecular assemblies of "porphysomes"[2-3] capable of undergoing active dissociation and releasing porphyrin moieties upon illumination, thereby enabling tunable photothermal properties with enhanced photodynamic efficiency. The new porphysomes are composed of smart phospholipid-porphyrin (PL-Por) conjugates that exhibit one or two ROS-responsive linkers separating the polar head group from the porphyrin moiety. Among the designed molecules, the monosubstituted conjugates with one porphyrin moiety showed the best performance in terms of stability, photothermal and photodynamic efficiencies in vitro. Moreover, these assemblies were found to achieve complete tumor ablation in 80% of PC3 prostate subcutaneous tumor-bearing mice, compared to 0% using conventional porphysomes. Besides cancer therapy, we demonstrated the efficiency of the new porphysomes in eradicating Gram + and Gram - bacteria as well as against their biofilm, with an improvement up to 10 folds in their antibacterial efficiency. Consequently, our strategy enabled the development of a versatile platform for delivering high payload of hydrophobic photosensitizers for enhanced photodynamic applications.

REFERENCES

[1] K. Merabishvili, I. Zmerli, J. Alhoussein, C. Regeard, A. Makky, *Chemical Society Reviews* **2025**, *54*, 8170-8195.
[2] J. F. Lovell, C. S. Jin, E. Huynh, H. Jin, C. Kim, J. L. Rubinstein, W. C. Chan, W. Cao, L. V. Wang, G. Zheng, *Nat. Mater.* **2011**, *10*, 324-332.
[3] J. Alhoussein, K. Merabishvili, T. Ho, A. Elkihel, P. Cressey, Á. Tóth, A. Qian, M. Hery, J. Vergnaud, S. Domenichini, F. Di Meo, J. Chen, G. Zheng, A. Makky, *Journal of Controlled Release* **2025**, *381*, 113621.

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Tripyridyl Porphyrin Derivatives and Their Photodynamic Action on Melanoma Cells under Hypoxic Conditions

Nela Malatesti[a], **Martina Mušković Lukić**[a], **Martin Lončarić**[b], **Nikola Basarić**[c], **Ivana Ratkaj**[a]

[a]*Faculty of Biotechnology and Drug Development, University of Rijeka, Radmile Matejčić 2, 51000 Rijeka, Croatia*
[b]*Laboratory for Photonics and Quantum Optics, Division of Experimental Physics, Ruđer Bošković Institute, Bijenička Cesta 54, 10000 Zagreb, Croatia*
[c]*Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička Cesta 54, 10000 Zagreb, Croatia*

Melanoma is the most dangerous form of skin cancer, with a high mortality rate if not detected early; it is characterised by a hypoxic tumour microenvironment that, through mechanisms not yet fully elucidated, allows rapid proliferation and migration of tumor cells, as well as resistance to various therapies [1]. The challenge of using photodynamic therapy (PDT) for the treatment of melanoma is twofold: hypoxia represents the primary obstacle, accompanied by the presence of melanin, which, due to its optical properties and antioxidant activity, protects tumor cells [2].
In our previous *in vitro* studies of AB_3 tripyridinium porphyrin derivatives with three *N*-methylated pyridyl groups (= B), the amphiphilic porphyrins with the longest (13, 15, and 17 C-atoms long) alkyl chains (amide-conjugated at the phenyl substituent = A) showed the highest uptake into melanoma cells and consequently the greatest PDT effect [3]. Therefore, we prepared analogous porphyrin derivatives with long chains, but with *N*-oxide groups instead of *N*-methyl groups, with the aim of investigating them as potential hypoxia-activated prodrugs (HAPs). All tested *N*-methylated pyridinium porphyrins showed significantly lower IC_{50} values after illumination on non-pigmented melanoma cells (A375) compared to pigmented melanoma cells (MeWo), and high selectivity for A375 cells relative to dermal fibroblasts (HDF), and they were also much less active in conditions of chemically induced hypoxia. On the other hand, porphyrins with *N*-oxide groups showed very similar PDT efficacy across all cell lines, and they were also found to be less sensitive to 'hypoxic' conditions induced by $CoCl_2$ [4].
Since $CoCl_2$ induces 'hypoxia' by stabilizing hypoxia-inducible factor 1α (HIF-1α), we are also studying the (photo)cytotoxicity of tripyridyl porphyrin derivatives with *N*-methyl or *N*-oxide moieties under conditions of reduced oxygen concentration using a hypoxia incubator chamber. Furthermore, using the B16F10 melanoma cell line with different melanin production (in different media), we are investigating the influence of this pigment on the PDT efficacy of our porphyrins. The (photo)physicochemical properties of these two groups of porphyrins, their uptake and localisation in cells, as well as the PDT effect on melanoma cells with different pigmentation, will be compared under conditions of normoxia and variously induced hypoxia, and discussed.

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REFERENCES

1. B. M. Robertson, M. E. Fane, A. T. Weeraratna, V. W. Rebecca, *Nature Cancer*, 2024, 5, 964–982.
2. L. Xin-Ying , T. Liu-Chang , D. Li-Wen , Z. Wan-Qi , S. Xiao-Xiao , L. Xiao , Z. Hong , L. Yuan-Gang, *Front. Oncol*. **2020**, 10, 597.
3. M. Mušković, M. Lončarić, I. Ratkaj, N. Malatesti, *Eur. J. Med. Chem*. **2025**, 282, 117063.
4. M. Mušković, M. Lončarić, I. Ratkaj, N. Malatesti, *Antioxidants*, **2025**, 14, 992.

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Towards Photoacoustic Imaging-Enabled Personalized Photodynamic Therapy: From Molecular Contrast to Real-time Oxygen Mapping

Srivalleesha Mallidi[a], **Andrew Langley**[a], **Ronak Shethia**[a], **Deeksha Sankepalle**[a], **Saad Mohammad**[b], **Tayyaba Hasan**[b]

[a]*Department of Biomedical Engineering, Tufts University, Medford MA USA*
[b]*Massachusetts General Hospital, Harvard Medical School, Boston MA USA*

Photodynamic therapy (PDT) is a clinically established, minimally invasive cancer treatment whose efficacy critically depends on photosensitizer distribution, light delivery, and, most importantly, the availability and dynamics of oxygen within the tumor microenvironment. However, the lack of robust, real-time dosimetry tools has limited the ability to personalize PDT and adapt treatment on the fly. Photoacoustic imaging (PAI), which combines optical contrast with ultrasound resolution and depth penetration, offers a unique opportunity to address this unmet need by enabling quantitative, spatially resolved monitoring of molecular agents and tumor physiology during therapy.

In this talk, we highlight how PAI can be leveraged as a powerful platform for personalized PDT dosimetry by integrating insights across molecular contrast mechanisms, oxygen dynamics, and advanced signal processing. First, we demonstrate that clinically relevant fluorophores and photosensitizers, such as IRDye800 conjugated to targeting antibodies, can serve as effective PA contrast agents. Importantly, PA signal exhibits distinct temporal dynamics compared to fluorescence, driven by aggregation state and intracellular processing, providing mechanistic insight into molecular binding, internalization, and degradation—parameters directly relevant to PDT timing. Second, we show that ultrasound-guided PAI enables real-time, spatially resolved monitoring of blood oxygen saturation (StO_2) during PDT, revealing heterogeneous oxygen consumption, fluence-rate–dependent hypoxia, and regions of reoxygenation that correlate with vascular function and long-term treatment response. Third, we discuss strategies to overcome practical limitations in molecular PA imaging, including photobleaching, using generative deep learning approaches that enable high-SNR, single-pulse imaging suitable for real-time clinical workflows. Finally, we present theranostic oxygen-carrying nanodroplets that synergistically enhance PDT efficacy while allowing direct PA monitoring of oxygen delivery and treatment response.

Collectively, these advances position photoacoustic imaging as a comprehensive, real-time dosimetry tool capable of informing PDT dose design, optimizing treatment timing, and enabling truly patient-specific photodynamic therapy.

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Imaging and Control of Microbial Metabolism by Targeting Extracellular Electron Transfer via Cytochrome Nanowires

Nikhil S. Malvankar[a]

[a]*Department of Molecular Biophysics and Biochemistry, Microbial Sciences Institute, Yale University*

ORALS

Every living cell must eliminate the surplus electrons produced by its metabolic processes. Most organisms achieve this by transferring electrons to soluble oxygen-like electron acceptors, which act as electron sinks. However, microbes that live in areas with limited or no oxygen, such as those in the deep ocean, soil, or the human body, have evolved strategies to export electrons to extracellular acceptors, including minerals or other bacteria. *Geobacter* uses hair-like conductive filaments called "nanowires" to export electrons [1-2]. Nanowires are fundamental to global environmental processes such as mineral and nutrient cycling, and have applications for bioremediation of toxic chemicals, bioenergy from waste and methane, and bioelectronics [3].

Geobacter nanowires have fascinated the scientific community since their discovery in 2002. Until recently, nanowires were considered heme-free proteins of Type IV pili (T4P). However, my lab showed that T4P is structurally inconsistent with electron transfer [4]. We further demonstrated that *Geobacter* produces additional filaments comprising polymers of outer membrane cytochrome (Omc) Z and S subunits, which can transfer electrons through a closely stacked (~5 Å) heme array [3, 5]. My lab showed that T4P functions as a piston to secrete cytochrome nanowires onto the bacterial surface. My team is exploring the structure, assembly, and electron transfer mechanism of nanowires, and evaluating their role in bacterial respiration and communication.
I will present our efforts to identify the mechanism underlying the highest electronic conductivity ever reported in proteins (>100 S/cm) [10]. Transient absorption spectroscopy and quantum dynamics simulations reveal ultrafast (<200 fs) electron transfer between nanowire hemes upon photoexcitation, enhancing carrier density and mobility.

By combining experimental and computational studies, our team is addressing three key questions:

- How do microbes kickstart metabolism [7] to build & use OmcS [6] & OmcZ [7] nanowires?
- How are electrons transferred from the bacterial cytoplasm to surface-displayed nanowires [8]?
- How to tune nanowire conductivity using light [9], pressure [10], temperature [11], electromagnetic fields [10], humidity [12], non-natural 'click' chemistry [13] & coherence [14] to control microbial behavior?

REFERENCES

1. Summers *et al.* Malvankar & Lovley, *Science* 2010
2. Malvankar *et al. Nature Nano.*, 2011 & *Nature Nano.*, 2014
3. Gu *et al.* Malvankar *Nature Micro.*, 2023
4. Gu *et al.* Malvankar *Nature*, 2021
5. Wang & Gu *et al.* Hochbaum, Egelman & Malvankar *Cell*, 2019
6. Shen *et al.* Malvankar *Cell Chemical Biology*, 2025
7. Erwin *et al.* Malvankar *Preprint*, 2024
8. Portela & Shipps *et al.* Malvankar, *Nature Comm.* 2024
9. Neu & Shipps *et al.* Malvankar, *Nature Comm*. 2022
10. Yalcin & O'Brien *et al.* Malvankar, *Nature Chem. Bio*., 2019
11. Dahl *et al.* Malvankar, *Science Adv.*, 2022
12. Dahl *et al.* Malvankar, *Preprint*, 2024
13. Shapiro *et al.* Malvankar & Isaacs, *Nature Comm.* 2022
14. Parson *et al.* Malvankar *JPCL*, 2025

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Photodynamic activity of novel porphyrin conjugates against bacteria in water

Muthumuni Managa, Mbalenhle K. Nhlabathi-Chidi, Knowledge S. Ndlovu and Malomane Nonkululeko

Institute for Nanotechnology and Water Sustainability (iNanoWS), Florida Campus, College of Science, Engineering and Technology, University of South Africa, Johannesburg 1710, South Africa

The fast-growing global population and contamination of water resources by human activities pose challenges to achieving clean, microbe-free water for drinking and domestic use. In most rural areas, water is stored in buckets or tanks, which can lead to biofilms. A biofilm comprises microorganisms in which cells stick to each other on a surface [1]. These adherent cells become embedded within a slimy extracellular matrix. Acquiring pure water free of contaminants (pollutants) and pathogens is a matter of concern, which calls for new, effective, and low-cost water disinfection techniques.

Antimicrobial photodynamic inactivation (aPDI) represents a potential alternative for inactivating microbial cells and has already been shown to be effective in vitro against bacteria, fungi, viruses, and protozoa [2]. There are various photosensitizers that have been developed for aPDI; the focus lies on porphyrinoids conjugated to nanostructured materials. Nanostructured materials have demonstrated desirable antimicrobial properties through various mechanisms, including inhibition of enzyme activity and photocatalytic production of reactive oxygen species to destroy the microorganisms [3]. This is due to the nanostructured materials having antimicrobial properties through their ability to carry photosensitizers. They provide multiple activation streams, including light and magnetic fields. Therefore, this will enhance the antimicrobial activity of the nanoconjugates

REFERENCES

1. López D, Vlamakis H and Kolter R. Cold Spring Harb. perspect. biol. 2010: 2, 1-11
2. Ndlovu KS, Chokoe K, Masebe T, Sekhosana KE, Moloto MJ, Managa M. Chemical Papers. 2024: 78:5004
3. Bhushan B, Luo D, Schricker SR, Sigmund W and Zauscher S. In “Handbook of Nanomaterials Properties”. Springer-Verlag, 2014, pp. 1053-1075

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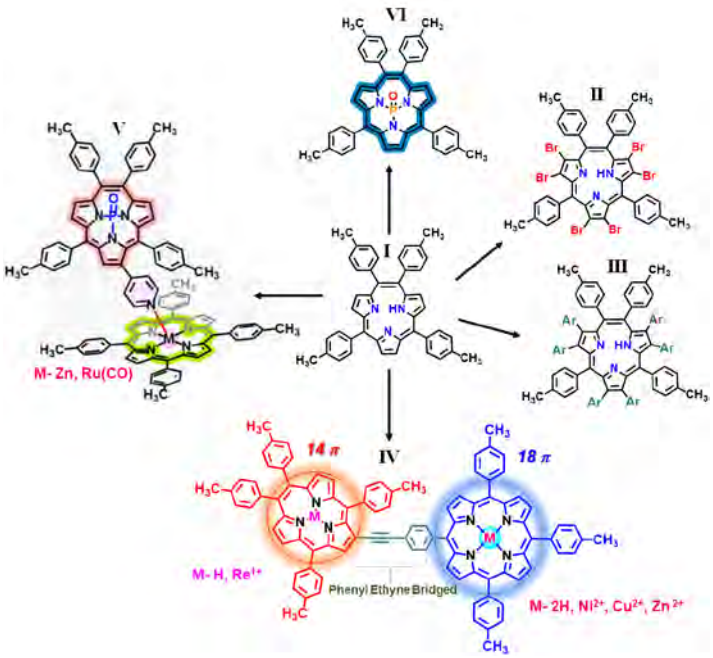
The Chemistry Of Newly Emerging Contracted 14 π Meso-Tetraaryl Triphyrin(2.1.1)s

M. Ravikanth[a]

[a]*Department of Chemistry, Indian Institute of Technology, Powai, Mumbai 400076, India*
E-mail: ravikanth@chem.iitb.ac.in

ORALS

Triphyrin(2.1.1)s are emerging contracted congeners of porphyrins containing three pyrrole rings connected *via* four *meso* carbons in 14π electron conjugation [1]. We developed facile route for the synthesis of meso-tetraaryl triphyrin(2.1.1)s and carried out different types of reactions to explore their reactivity. The chemistry of these new contracted 14π triphyrin(2.1.1)s will be discussed in my presentation.



REFERENCES

1. Panda, K. N.; Thorat, K. G.; Ravikanth, M. *J. Org. Chem.* **2018**, *83*, 12945-12950.
2. Alka, A.; Ravikanth, M. *J. Org. Chem.* **2021**, *86*, 17640-17650.
3. Sharma, A.; Alka, A.; Ravikanth, M. *Chem. Asian J.* **2024**, *19*, e202400799.
4. Sharma, A.; Alka, A.; Ravikanth, M. *Chem. Asian J.* **2025**, *20,* e70477.
5. Sharma, A.; Ravikanth, M. *Dalton Trans.* **2025**, *54*, 6935-6945.
6. Maji, A.; Sharma, A.; Ravikanth, M. *Inorg. Chem.* **2026**,(In press).

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A High Valent Mn(V)-Nitrido Species within a *De Novo* Designed Protein

Samuel I. Mann[a], **Jithin Thomas**[a], **Sudha Yadav**[b], **Paul H. Oyala**[c], **Veronica Carta**[a], **David P. Goldberg**[b]

[a] *Department of Chemistry, University of California, Riverside, Riverside, CA, USA*
[b] *Department of Chemistry, The Johns Hopkins University, Baltimore, MD, USA*
[c] *Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, USA*

High-valent metal-oxo species are ubiquitous oxidants in chemical and biological systems, however their metal-nitrido analogues remain far less explored, particularly in a biological context, due to challenge associated with instability and bimolecular N-N coupling. Here, we report the first example of a high-valent metal-nitrido species within a *de novo* designed protein scaffold. A Mn(V)-nitrido complex derived from an abiological diphenyl porphyin was generated and confined within a designed helical bundle protein, where the protein environment suppresses bimolecular decay. Spectroscopic characterization, including electron paramagnetic resonance (EPR), resonance Raman(rR), and circular dichroism (CD) confirms the formation of a low-spin Mn(V)≡N species that is stable for weeks at room temperature and shows no effect from the axial histidine (His) ligand. We hypothesize that monochloramine (NH_2Cl), generated using NH4OH/NaOCl, is the active species responsible for formation of a reactive intermediate en-route to the nitrido and show that we can intercept this reactive intermediate for the first enantioselective aziridination by a de novo protein. Importantly, this work establishes *de novo* protein design as a platform for accessing metal-nitrido chemistry that has no known biological precedent.

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A fire toxic gases injectable antidote composed of synthetic porphyrins

Qiyue Mao[a], **Hiroaki Kitagishi**[a]

[a]*Faculty of Science and Engineering, Department of Molecular Chemistry and Biochemistry, Doshisha University*

ORALS

During fires, 2 highly toxic components of smoke, carbon monoxide (CO) and hydrogen cyanide (HCN), are produced simultaneously, and more than 50% of fire-related deaths can be attributed to their inhalation. CO binds to ferrous heme, and HCN binds to ferric heme, which is one of the key mechanisms by which CO and HCN perform their toxicological mechanisms. Because of their differing detoxification mechanisms, there is currently no method to detoxify them simultaneously. In our group, a supramolecular complex named hemoCD-P (Fig. 1A) has been used for several years to investigate the physiology of endogenous CO.[1] HemoCD is the first aqueous synthetic hemoglobin (Hb) model complex that is supposed to show similar gas binding ability to Hb. We also reported another hemoCD type, hemoCD-I (Fig. 1A), which can capture cyanide *in vivo*. [1] On this basis, we developed an injectable antidote that can remove CO and HCN simultaneously from the body by mixing the two different hemoCD analogues (hemoCD-Twins).[2] hemoCD-Twins exhibits rapid, simultaneous CO and HCN detoxification, with good safety and excellent storage stability. In this presentation, the strategy of using hemoCD-Twins as an injectable antidote for fire-toxic gas poisoning will be presented.

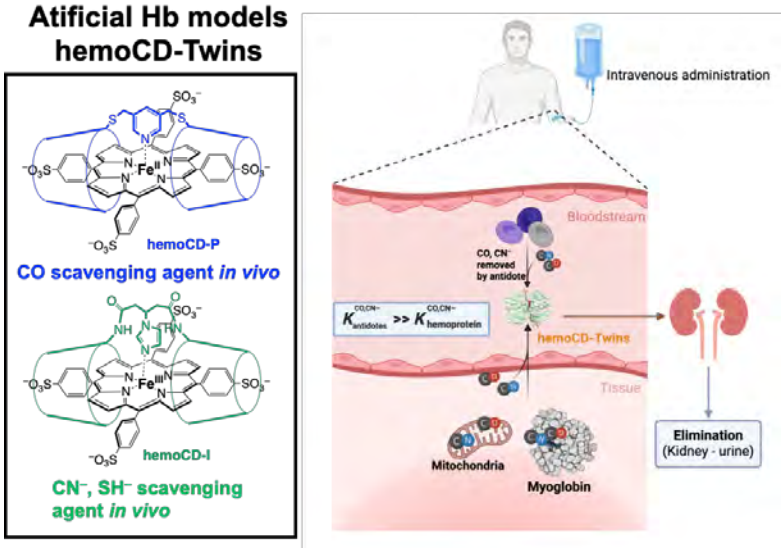


Fig 1. (A) Structures of hemoCD-P and hemoCD-I. (B) The strategy of using hemoCD-Twins as an injectable antidote for fire toxic gases poisoning.

REFERENCES

(1) H. Kitagishi, et al. *Chem Comm*, **57**, 148–173 (2021). (2) Q. Mao, et al. *Proc. Natl. Acad. Sci. U.S.A.*, **120**, e2209924120 (2023).

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Unconventional Pnictogen–Nitrogen Species as Building Blocks for Molecular Materials

Artur Mardyukov

[a] *Justus Liebig University Giessen, 35392 Giessen, Germany. Email: artur.mardyukov@org.chemie.uni-giessen.de*

ORALS

Molecular main-group species with unconventional bonding motifs offer powerful opportunities for the bottom-up design of functional molecular and low-dimensional materials. In this contribution, we present controlled synthetic access to reactive pnictogen–nitrogen species and nitrogen allotropes that serve as fundamental molecular building blocks. We demonstrate the formation of an o-benzoquinone–PN complex generated by UV irradiation (λ = 254 nm) of (o-phenyldioxyl)phosphinoazide under cryogenic conditions. Subsequent green-light irradiation (λ = 523 nm) induces reversible recombination to (o-phenyldioxyl)-λ⁵-phosphinonitrile, representing the first experimentally verified interaction of phosphorus mononitride (PN) with an organic π-system.[1] Extending this strategy to heavier congeners, we report the selective generation and spectroscopic characterization of arsenic mononitride (As≡N), a long-elusive molecular precursor to arsenic–nitrogen materials with emerging semiconducting relevance (Figure 1A).[2]

We further describe the on-surface synthesis of cyclotriphosphazene (P_3N_3), an inorganic aromatic analogue of benzene, achieved by voltage-pulse-induced dechlorination of $P_3N_3Cl_6$ on Cu(111) at 5.2 K, with real-space imaging confirming its planar D_{3h} symmetry (Figure 1B).[3] Finally, we report the synthesis of neutral hexanitrogen (N_6), a long-sought nitrogen allotrope, obtained via gas-phase halogenation of silver azide and stabilized by cryogenic isolation, exhibiting unexpected kinetic stability.[4] Together, these results establish pnictogen–nitrogen molecules as versatile platforms for molecular materials with unconventional electronic structures (Figure 1C).

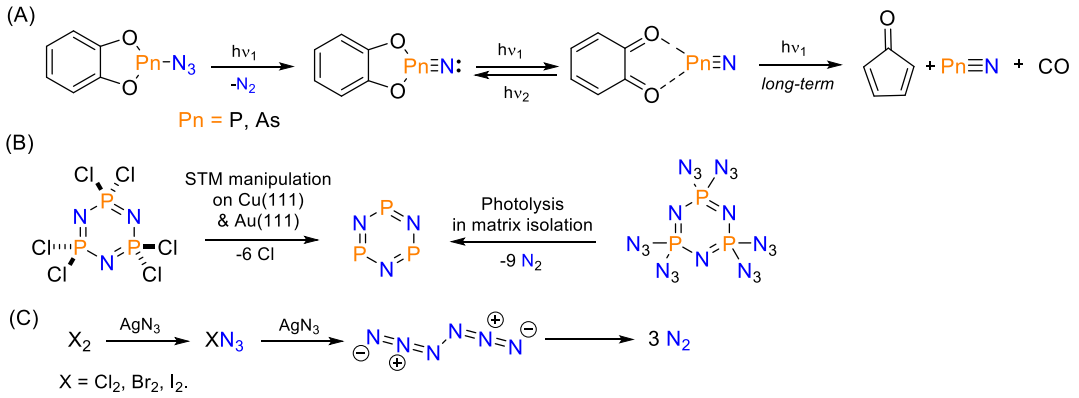


Figure 1. Reaction sequences employed in the studies.

1. W. Qian, R. C. Wende, P. R. Schreiner, A. Mardyukov, Angew. Chem. Int. Ed., 2023, 62, e202300761.
2. W. Qian, R. C. Maria Eugenia Sandoval-Salinas, Rachel Crespo-Otero, Peter R. Schreiner, Artur Mardyukov, JACS, 2026, accepted.
2. Q. Zhong, A. Mardyukov, E. Solel, D. Ebeling, A. Schirmeisen, P. R. Schreiner, Angew. Chem. Int. Ed., 2023, 62, e202310121.
3. W. Qian, A, Mardyukov, P. R. Schreiner, Nature, 2025, 642. 356–360.

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Excited charge separation in silicon(IV) phthalocyanine with axially bound C_{60} via azobenzene spacers

Luis Martín-Gomis[a], Andrew W. Dawson[b], Victor Sobrino-Bastán[a], Francis D'Souza[b] and Ángela Sastre-Santos[a]

[a] *Área de Química Orgánica, Instituto de Bioingeniería, Universidad Miguel Hernández, Avda Universidad S/N, 03202, Elche, Spain.*
[b] *Department of Chemistry, University of North Texas, 1155 Union Circle, # 305070, Denton, Texas 76203-5017, USA*

ORALS

Artificial photosynthesis fundamentally involves designing molecular architectures capable of converting light energy into chemical or electrical potential, a process that necessitates highly efficient donor-acceptor systems 1]. Phthalocyanines (Pcs), specifically the versatile silicon(IV) phthalocyanine (SiPc), owing to its hexacoordination capability, function as robust electron donors [2], while C_{60} fullerenes are recognized as potent electron acceptors [3]. However, a critical challenge for the practical implementation of these systems, such as in organic photovoltaics, remains the achievement of charge-separated (CS) states with lifetimes exceeding the nanosecond regime.

This communication presents a novel donor-acceptor triad, C_{60}-azo-SiPc-azo-C_{60} (**Figure 1**) 4], incorporating two C_{60} units axially bound to the SiPc core via azobenzene (azo) spacers, components known for their ability to dynamically modulate electronic properties and intermolecular distance. The nanosecond transient absorption analysis established that the $SiPc^{\bullet+}$-$C_{60}^{\bullet-}$ charge-separated state exhibits long lifetimes, exceeding those measured for previous non-azo analogues, suggesting its potential for further photocatalytic and optoelectronic applications.

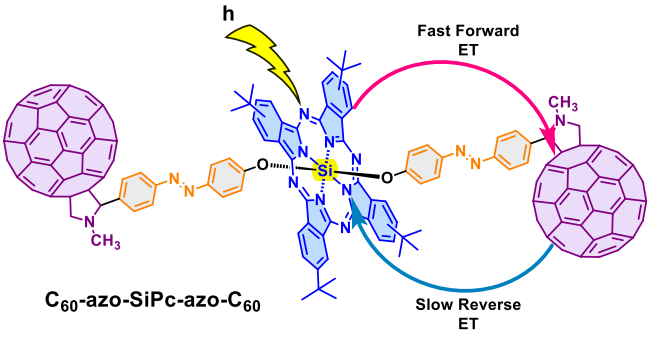


Figure 1. Chemical structure of C_{60}-azo-SiPc-azo-C_{60} triad.

REFERENCES

1 Wang Z, Hu Y, Zhang S and Sun Y. *Chem. Soc. Rev.* 2022; **51**: 6704-6737.
2 Bottari G, De La Torre G, Guldi DM and Torres T. *Chem. Rev.* 2010; **110**: 6768-6816.
3 Martín-Gomis L, Seetharaman S, Herrero D, Karr PA, Fernández-Lázaro F, D'Souza F and Sastre- Santos Á. *ChemPhysChem* 2020; **21**: 2254–2262.
4 Dawson AW, Sobrino-Bastán V, Martín-Gomis L, Sastre-Santos Á and D'Souza F. *J. Porphyrins Phthalocyanines* 2025; **29**: 1093-1106.

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New Challenges in Chiral Subphthalocyanines

M.V. Martinez-Diaz,[a,b] L. Tejerina,[a] G. Lavarda,[a] M. Lahoz,[a] R. de Miguel,[a] J. Garcia-Calvo,[a,b] P. de la Rubia,[a] and T. Torres[a,b,c]

[a]*Departamento de Química Orgánica, Universidad Autónoma de Madrid, 28049 Madrid*
[b]*Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid, Spain.*
[c]*IMDEA Nanociencia, C/Faraday, 9, Cantoblanco, 28049 Madrid, Spain.*

Owing to their peculiar curved shape, "bowl" chirality is an inherent property of certain SubPcs when, adequately functionalized at the peripheral positions, the macrocycle lacks a mirror plane [1]. Moreover, they exhibit high bowl inversion barriers, which have enabled the separation of small quantities of the *M* and *P* enantiomers by chiral column chromatography [2]. Namely, both enantiomers of chiral C_3-symmetric SubPcs bearing peripheral halogens (bromine, iodine) atoms have been resolved by semi-preparative chiral HPLC [3] in sufficient amount to study properties derived from chirality such as spin polarization [4]. However, the intrinsic limitations of the HPLC technique (low throughput, high cost, and time-consuming multiple runs and method development), together with specific solubility issues of the SubPc framework, hamper scalability and feasibility, thereby hindering the exploitation of curved SubPc aromatics as chiral materials. On the other hand, the exploration of alternative procedures (namely, chiral resolution with chiral auxiliaries or *de novo* asymmetric synthesis) for the preparation of enantiopure SubPcs by common organic laboratory techniques remains a pending task. Here, we report the efficient optical resolution of inherently chiral C_3-symmetric SubPcs *via* axial derivatization with BINOL-based chiral auxiliaries [5]. In addition, a new way of inducing chirality in SubPc should be the result of fusing chiral binaphthyl or biphenantryl units to the macrocyclic core [6].

REFERENCES

1. C. G. Claessens and T. Torres, Tetrahedron Lett., 2000, 41, 6361–6365.
2. J. Guilleme, M. J. Mayoral, J. Calbo, J. Arago, P. M. Viruela, E. Orti, T. Torres and D. Gonzalez-Rodriguez, Angew. Chem. Int. Ed., 2015, 54, 2543 –2547.
3. J. Labella, G. Lavarda, L. Hernández-López, F. Aguilar-Galindo, S. Díaz-Tendero, J. Lobo-Checa and T. Torres, J. Am. Chem. Soc., 2022, 144, 16579−16587.
4. J. Labella, D. K Bhowmick, A. Kumar, R. Naaman and T. Torres, Chem. Sci., 2023, 14, 4273–4277.
5. G. Lavarda, L. Tejerina, T.Torres and M. V. Martinez-Diaz, Chem. Sci., 2024, 15, 19369–19374.
6. L. Zhao, D. Qi, K.Wang, T.Wang, B. Han, Z. Tang, and J. Jiang, Sci. Reports, 2016, 6, 28026.

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Mechanistic insights into carbene transfer catalyzed by transition metal tetrapyrroles: bridging spectroscopy and theory

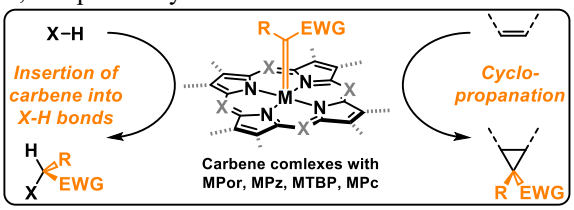
Alexander G. Martynov[a], Andrey P. Kroitor[a], Alexander A. Dmitrienko[a], Yulia G. Gorbunova[a,b], Alexander B. Sorokin[c]

[a]*Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, Moscow, Russia*
[b]*Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, Moscow, Russia*
[c]*Institut de Recherches sur la Catalyse et l'Environnement de Lyon, IRCELYON, UMR 5256, CNRS – Université Lyon 1, Villeurbanne, France*

ORALS

Various macrocyclic ligand-based transition metal complexes are commonly used as catalysts for carbene transfer, which enables the efficient construction of a diverse range of functionalized molecules, including valuable biologically active compounds and pharmaceutical intermediates. While porphyrin-based catalysts dominate this field, other tetrapyrrolic scaffolds remain underexplored, offering a rich design space for novel catalytic properties and activities [1-4].

To systematically broaden the scope of tetrapyrrolic carbene-transfer catalysts by moving beyond the porphyrin paradigm we conducted a comprehensive comparative study of the catalytic activity of Mn(III), Fe(III), Co(II), Cu(II), and Ru(II) complexes supported by a series of distinct macrocyclic ligands including porphyrazines, benzoporphyrins, and phthalocyanines.



These complexes were evaluated in model carbene-transfer reactions between diazo compounds and various substrates (e.g., styrenes, amines, silanes). Our screening revealed a pronounced "ligand-effect," where the identity of the tetrapyrrolic scaffold dramatically modulates the activity of a given metal ion, underscoring the critical role of the coordination environment beyond the central metal.

To rationalize these observed differences, we employed a synergistic combination of spectroscopic techniques and quantum-chemical calculations. This approach allowed us to identify key reactive intermediates and model potential reaction pathways. In this talk, we will present compelling examples of this combined analysis, demonstrating how the electronic and geometric structure of the macrocycle dictates catalytic performance and opens new avenues for catalyst design.

Acknowledgement: this work was supported by Russian Science Foundation, project № 25-13-00332

REFERENCES

1. Cailler LP et al. *Inorg. Chem.* 2020; **59**: 1104-1116.
2. Kroitor AP et al. *Org. Biomol. Chem.* 2023; **21**: 69-74.
3. Kroitor AP et al. *ACS Catal.* 2025; **15**: 4984-5001.
4. Dmitrienko AA et al. *J. Catal.* 2025; **452**: 116443.

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The structure-function relationship of heme sensor proteins

Markéta Martínková, Artur Sergunin, Petr Pompach, Jakub Vávra, Dominik Pašek, Toru Shimizu

Department of Biochemistry, Faculty of Science, Charles University, Hlavova 2030-8, Prague 2, Czech Republic

A wide range of physiological and pathological processes in many organisms, including humans, are influenced by the heme molecule. The regulatory role of heme is mediated by a group of proteins known as heme sensor proteins. It is well established that heme can function either as a signaling molecule itself or as a gas-sensing cofactor in heme-based gas sensors [1]. Understanding the structure–function relationships of heme sensor proteins is therefore a particularly important area of research. Clearly, the function of heme sensor proteins is closely linked to their structure, which is, in turn, modulated by signal sensing. However, this relationship is often more complex, as many heme sensor proteins—or at least certain domains or regions within them—exhibit intrinsically disordered conformations. A key challenge is to elucidate the molecular mechanisms underlying their sensing functions and signal transduction.

Signal transduction in a representative bacterial heme-based oxygen sensor is discussed using the example of the globin-coupled histidine kinase (AfGcHK) from Anaeromyxobacter sp. strain Fw109-5. In this dimeric sensor protein, the dimerization interface of the sensing domain plays a crucial role in signal transmission. This mechanism is compared with signal transduction in a classical human heme sensor, the heme-regulated eukaryotic initiation factor 2α (eIF2α) kinase, also known as the heme-regulated inhibitor (HRI), which undergoes substantial conformational changes upon heme binding [3].

The family of human heme-sensing proteins has recently expanded with the identification of numerous new members. Among these, a direct signaling role for heme has been demonstrated in a tumor suppressor p53, a central regulator of cellular stress responses [4]. p53 is a transcription factor that preserves genomic integrity and prevents tumor development. Upon activation, it binds to DNA and regulates a broad network of genes involved in apoptosis, cell-cycle arrest, DNA repair, senescence, and metabolism. Loss or functional inactivation of p53 is one of the most common hallmarks of human malignancies. In this study, we aimed to characterize the structural consequences of the interaction between heme and p53. Using hydrogen–deuterium exchange mass spectrometry on full-length p53, we found that the DNA-binding domain undergoes the most pronounced conformational changes upon heme binding. These alterations likely explain the previously reported heme-induced functional inhibition of p53 [5]. We further extended our analysis to p63, another member of the p53 protein family, and demonstrated that full-length p63 also directly interacts with heme. Despite the significant structural and functional similarities between p53 and p63, our results indicate that heme interacts differently with their full-length forms. Nevertheless, in both proteins, heme binding led to destabilization and aggregation of the isolated DNA-binding domains, suggesting a shared mechanism of heme-induced misfolding. Together, these findings establish an important link between heme signaling and the structural regulation of p53 family proteins, with broader implications for understanding cancer progression and for the development of novel therapeutic strategies targeting heme–protein interactions. Supported by the Grant Agency of the Czech Republic (grant 177424).

REFERENCES

1. Shimizu et al., 2019, Chem. Soc. Rev. 48: 5624.
2. Skalova et al., 2020, J. Biol. Chem. 295: 1587.
3. Igarashi et al., 2008, J. Biol. Chem. 283: 18782.
4. Shen et al., 2014, Cell Rep. 7:180.
5. Vávra et al., 2023, J. Inorg. Biochem. 243:112180.

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Development of Molecular Catalysts for Photosynthetic Reactions

Shigeyuki Masaoka[a]

[a]*Division of Applied Chemistry, Graduate School of Engineering, The University of Osaka*

ORALS

Photosynthesis is a biochemical process that converts carbon dioxide and water into carbohydrates while simultaneously storing solar energy as chemical energy in the products. In natural photosynthesis, solar energy is first converted into electrochemical energy through charge separation, and the resulting electrochemical potentials drive multi-electron redox reactions of small molecules. Inspired by these processes, our group has been investigating the development of molecular catalysts for electrochemical and photochemical small-molecule conversions involving multi-electron transfer. Such studies are expected to contribute to the solution of global energy and resource challenges. Recent achievements from our group include: (i) development of pentanuclear metal complexes as active centers for electrochemical or photoochemical small-molecule conversions [1-4], (ii) investigations of electrochemical or photochemical insertion reactions of small molecules into low-reactivity organic substrates [5-7], and (iii) the construction of highly efficient catalytic systems based on metal complexes for molecular conversions [8-11].

REFERENCES

1. M. Okamura, M. Kondo, S. Masaoka *et al.*, *Nature*, **2016**, *530*, 465–468.
2. M. Kondo, S. Masaoka, *Acc. Chem. Res*. **2020**, *53*, 2140–2151.
3. H. Izu, M. Kondo, S. Masaoka *et al.*, *Angew. Chem. Int. Ed.*, **2024**, e202408514.
4. T. Matsuzaki, K. Kosugi, M. Kondo, S. Masaoka *et al.*, *Nat. Commun.*, **2025**, *16*, 2145.
5. Y. Morii, T. Watanabe, Y. Saga, S. Masaoka *et al.*, *ChemElectroChem*, **2024**, *11*, e20240006.
6. T. Watanabe, Y. Saga, S. Masaoka *et al.*, *Org. Lett.*, **2024**, *26*, 6491–6496.
7. P. Lorwongkamol, Y. Saga, S. Masaoka *et al.*, *JACS Au*, **2025**, *5*, 4170–4177.
8. S.-K. Lee, M. Kondo, S. Masaoka *et al.*, *J. Am. Chem. Soc.*, **2018**, *140*, 16899–16903.
9. K. Kosugi, M. Kondo, S. Masaoka, *Angew. Chem. Int. Ed.*, **2021**, *60*, 22070–22074.
10. H. Iwami, M. Kondo, S. Masaoka *et al.*, *Angew. Chem. Int. Ed.*, **2021**, *60*, 5965–5969.
11. K. Kosugi, M. Kondo, S. Masaoka *et al.*, *J. Am. Chem. Soc.*, **2023**, *145*, 10451–10457.

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Nanomaterial-porphyrinoid composites as excellent electrochemical sensors

Philani Mashazi, Tebogo Mpakanyane, Lunathi Ncwane, Tebello Nyokong

Institute for Nanotechnology Institute, Rhodes University, PO Box 94, Makhanda, 6139 South Africa

Nanomaterial-porpyrinoid conjugates and composites are explored for their excellent electrochemical application for the detection of various compounds on health and environmental importance. In the recent past we have studied nanomaterials composites with covalent (COMFs) and metal (MOMFs) organic macrocycle frameworks as electrode modifiers. These were modified onto glassy carbon electrode as for electrochemical sensing of water pollutants and disease biomarkers.

Here, cobalt(II)-porphyrin conjugated microporous polymer (CoPor-Tp-CMP) was integrated with reduced graphene oxide (rGO) and functionalized single-walled carbon nanotubes (fSWCNTs) to create a hybrid materials (CoPor-Tp-CMP/rGO and CoPor-Tp-CMP/fSWCNTs) electrodes with enhanced electrocatalytic performance [1]. The CoPor-Tp-CMP provided high surface area and abundant redox-active sites, while fSWCNTs and rGO contributed excellent conductivity and rapid electron transfer, enabling dimensional tuning and π–π stacking interactions. A cobalt(II)-cobalt(II) octacarboxy phthalocyanine (Co-CoOCPc-MOFs) based metal organic macrocycle frameworks (MOMFs) were composited silver nanoparticles (AgNPs) to form Co-CoOCPc-MOFs/AgNPs electrodes with anti-HER2 aptamer electrodes. The electrodes were used for ultrasensitive detection of a cancer biomarker, human epidermal growth factor receptor 2 (HER2) [2]. The prepared materials were studied and characterized using various techniques which confirmed the successful preparation and integration onto glassy carbon electrode (GCE) surface. The results on these studies shed information of how the COFs and MOFs of composites pophyrinoid materials are effective as electrode materials and for sensing applications.

REFERENCES

1. Teboho Edwin Mpakanyane, Philani Mashazi, Tebello Nyokong, Metalloporphyrin-conjugated microporous polymer-carbon materials hybrids for highly sensitive electrochemical detection of 4-hydroxybenzoic acid, *Dyes and Pigments* 246 (**2026**) 113300.

2. Lunathi Ncwane, Philani Mashazi, Tebello Nyokong, Phthalocyanine based metal organic frameworks for electrochemical detection of human epidermal growth factor receptor 2, *Bioelectrochemistry* 165 (**2025**) 108966.

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Construction of stable myoglobin oligomers by designed 3D domain swapping

Tsuyoshi Mashima[a,b], **Haruki Onishi**[a], **Yuya Tanaka**[a], **Naoya Kobayashi**[a], **Shun Hirota**[a,b]

[a]*Graduate School of Science and Technology, Nara Institute of Science and Technology*
[b]*Medilux Research Center, Nara Institute of Science and Technology*

ORALS

In nature, protein assemblies play important roles in biomolecule production, storage, transfer, etc. Recently, protein assemblies have been constructed as new functional biomaterials, increasing the importance of oligomerization methods that can stably form desired protein oligomeric structures. We previously showed that myoglobin (Mb), which consists of eight α-helices (A–H), dimerizes via 3D domain swapping (3D-DS) wherein the same structural region is exchanged three-dimensionally between molecules of the same protein.[1] The hinge loop between helices E and F converted to a helical structure and merged with helices E and F to form one extended α-helix. In this study, we aimed to induce dimerization through 3D-DS by modifying a helix-loop-helix motif into a single continuous helix at a target site. Specifically, we substituted the GH loop region of Mb with reported α-helical linkers (Fig. 1). We designed 21 variants of Mb (Mb1–Mb21) and successfully obtained two dimeric variants, Mb3 and Mb8. X-ray crystallographic analysis revealed that the GH loop region in both variants form an α-helix, leading to dimerization via 3D-DS. However, both variants showed reduced thermal stability compared to that of wild-type Mb and existed in equilibrium between monomeric and dimeric forms. To stabilize the dimeric structure, the surface and the inserted helical linker segments of Mb3 were redesigned with ProteinMPNN. Six redesigned Mb variants (reMb3A–F) were expressed in E. coli, and five of them were obtained exclusively as dimers as soluble components. reMb3B, which showed the highest expression level, was analyzed by X-ray crystallography, revealing a dimeric structure similar to that of Mb3. The melting temperature of reMb3B was higher than that of Mb3 for more than 20 °C. In addition, we constructed Mb oligomers via continuous 3D-DS by combining designed 3D-DS at the EF-loop and GH-loop regions.

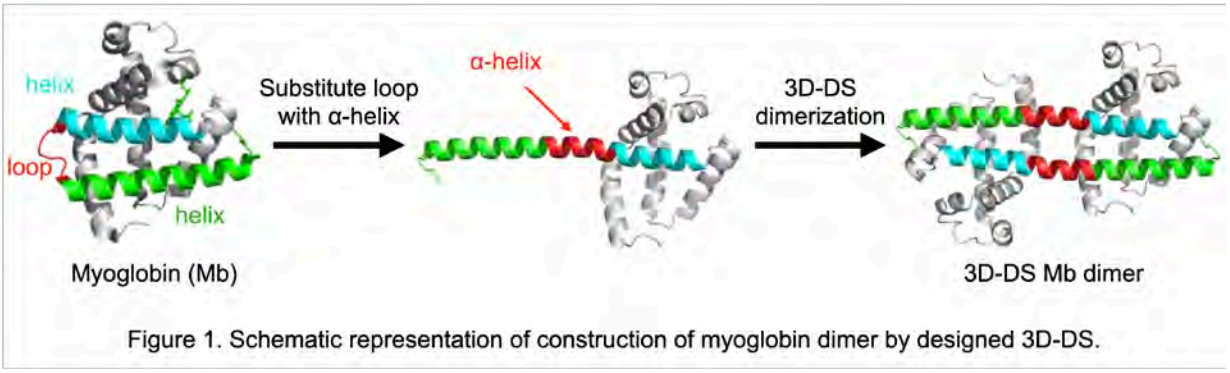


Figure 1. Schematic representation of construction of myoglobin dimer by designed 3D-DS.

REFERENCES

1. S. Hirota, et al., *Dalton Trans.*, **2012**, *41*, 11378–11385.

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Trafficking of Heme as Plastid-Derived Retrograde Signal in Plant Cells

Mihoko Takenoya[a], Takayuki Shimizu[b], Tatsuru Masuda[a]

[a]*Graduate School of Arts and Sciences, The University of Tokyo*
[b]*Faculty Divisions of Natural Sciences, Nara Women's University*

In plant cells, heme is synthesized in plastids and metabolized to phytochromobilin (PΦB) in two enzymatic steps: heme oxygenase (HO) and PΦB synthase (HY2), which is coupled to the functional phytochrome assembly. In addition, heme is trafficked to various organelles as a cofactor for hemoproteins and as a plastid-derived retrograde signal in the control of photosynthesis-related nuclear gene (*PhANG*) expression. We discovered that the localization of the predominant *Arabidopsis* HO isoform, HO1, is altered in plastids or the cytosol due to transcriptional start site regulation, and heme metabolism occurs not only in plastids but also in the cytosol [1]. The later HY2 reaction can also be performed in the cytosol by alternative splicing in which the 1st intron retention produces the cytosolic HY2. By complementing the *genomes uncoupled* (*gun*) phenotype, we revealed that the cytosolic heme degradation was effective in canceling the signaling function of heme for *PhANGs* regulation. By introducing regiospecific bacterial HOs, we further demonstrated that a plastid-derived retrograde mobile heme signal passing through the cytosol is independent of the phytochrome-dependent light signaling [2].

For heme trafficking, ABC transporters are proposed to be involved in the transport of heme out of plastids, which allows it to pass through the membrane. We identified *AtABCG23* in *Arabidopsis* by comprehensive proteomic analysis of heme-binding proteins [3]. Since *AtABCG23* showed gene redundancy due to forming a gene family, we produced a quadruplet mutant of *atabcgq* and analyze it. We also identified the *AtABCG23* homolog from *Marchantia polymorpha*, which has one copy of the ancestral gene (*MpABCG23*). AtABCG23 and MpABCG23 were localized in the chloroplast envelope membrane. Transport experiments using proteoliposomes revealed that both transported the heme analog Zn-protoporphyrin IX in an ATP-dependent manner with high substrate specificity for heme. Functions of the *AtABCG23* family and *MpABCG23* will be discussed in the presentation.

REFERENCES

1. Chen et al. (2024) *Plant Physiol.* 195 : 2937.
2. Takenoya et al. (2025) *in preparation.*
3. Shimizu et al. (2020) *Phil Trans R Soc Lond B Biol Sci.* 375 : 20190488.

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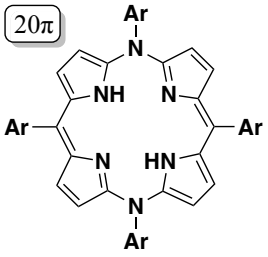
Azaporphyrinoids Bearing *meso*-N-Substituents: Platforms for Evaluating Antiaromaticity and Aromaticity

Yoshihiro Matano

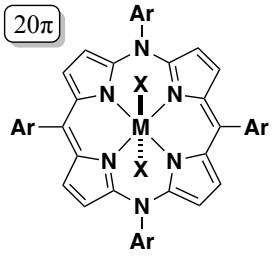
Department of Chemistry, Faculty of Science, Niigata University, Japan

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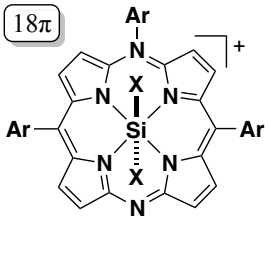
The 2e-reduced species of regular porphyrins, 20π-electron porphyrins, are inherently antiaromatic macrocycles, and their structure–property relationship has long been a subject of interest for understanding the key factors that govern their antiaromaticity and optical properties. To avoid the use of extremely air- and moisture-sensitive porphyrin dianions, several elaborate strategies have been adopted to isolate neutral 20π-electron porphyrinoids.[1] Our group has reported metal complexes of 5,10,15,20-tetraaryl-5,15-diazaporphyrinoid (Ar_4DAP) that are obtained by the metal-templated cyclization of the corresponding metal–bis(dipyrrin) complexes.[2] Recently, our group has also established a general method for the synthesis of freebases (Ar_4DAPH_2 **1**) and converted **1** to hexacoordinate silicon(IV) and tin(IV) complexes ($Ar_4DAPSiX_2$ **2** and $Ar_4DAPSnX_2$ **3**).[3] In contrast to the isoelectronic 20π-electron TPP-type porphyrinoids, **1**, **2** and **3** are extremely air stable in the solid state. We have also prepared silicon(IV) complexes of 5,10,20-triaryl-5,15-diazaporphyrinoids ($Ar_3DAPSiX_2$ **4**)[4] and 5,10,15,20-tetraaryl-5-monoazaporphyrinoid ($Ar_4MAPSiX_2$ **5**),[5] which are cationic in the 18π-electron state. In this presentation, the synthesis, structures, optical and redox properties, and antiaromatic/aromatic characters of these azaporphyrinoids are reported.



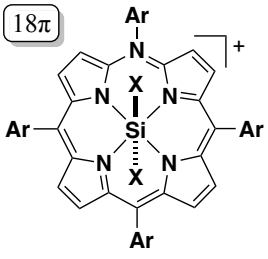
Ar_4DAPH_2 **1**



$Ar_4DAPSiX_2$ **2** (M = Si)
$Ar_4DAPSnX_2$ **3** (M = Sn)



$Ar_3DAPSiX_2$ **4**



$Ar_4MAPSiX_2$ **5**

REFERENCES

1. a) K. Reddy, A. Basavarajappa, M. D. Ambhore, V. G. Anand, *Chem. Rev.* **2017**, *117*, 3420. b) Y. Matano, *Handbook of Porphyrin Science*, Eds. K. M. Kadish, K. M. Smith, R. Guilard, World Scientific, **2022**, Vol. 46, Chap. 219, pp. 41–111.
2. a) T. Satoh, M. Minoura, H. Nakano, K. Furukawa, Y. Matano, *Angew. Chem. Int. Ed.* **2016**, *55*, 2235. b) K. Sudoh, T. Satoh, T. Amaya, K. Furukawa, M. Minoura, H. Nakano, Y. Matano, *Chem. Eur. J.* **2017**, *23*, 16364. c) H. Ochiai, K. Furukawa, H. Nakano, Y. Matano, *J. Org. Chem.* **2021**, *86*, 2283.
3. a) H. Suzuki, K. Furukawa, M. Minoura, H. Nakano, Y. Matano, *Bull. Chem. Soc. Jpn*, **2024**, *97*, uoad022. b) H. Suzuki, M. Minoura, K. Furukawa, H. Nakano, Y. Matano, *Chem. Eur. J.* **2025**, *31*, e202404092.
4. K. Sasaki, Y. Murata, H. Suzuki, M. Minoura, R. Kitakado, Y. Kimura, K. Furukawa, H. Nakano, Y. Matano, et al., *J. Porphyrins Phthalocyanines* **2025**, *29*, 467.
5. K. Sasaki, Y. Murata, M. Minoura, H. Nakano, Y. Matano, manuscript in preparation.

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Biomaterials based on Porphyrinoid/Cyclodextrin Assemblies: from Hybrids to Composites with Photoantimicrobial Action

Giuseppe Nocito[a], Giuseppe Mistretta[a,b], Mariachiara Trapani[a], Simona Salerno[c], Roberto Zagami[b], Luigi Monsù Scolaro[b] and Antonino Mazzaglia[a]

[a]National Research Council, Institute for Nanostructured Materials (CNR-ISMN), URT of Messina at Department of Chemical, Biological, Pharmaceutical and Environmental Sciences (ChiBioFarAm), University of Messina, Viale F. Stagno d'Alcontres 31, 98166 Messina,[b]Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, V.le F. Stagno d'Alcontres 31, 98166, Messina, Italy
[c]National Research Council, Institute on Membrane Technology (CNR-ITM), Via P. Bucci 17/c, 87036 Rende (CS), Italy

ORALS

The rapid rise in antimicrobial resistance (AMR) demands innovative and broad-spectrum antimicrobial solutions capable of inactivating pathogens without favouring resistance development. Within our ongoing research on photosensitising supramolecular assemblies [1], here we present various novel biomaterials based on cyclodextrin and porphyrinoids to fight infections. In particular, we discuss assemblies of (Zn(II)- meso Tetra (N-methyl-4-pyridyl)-21*H*,23*H*-porphyrin Tetratosylate (ZnT4)) with the trade sulfobutylether-β-cyclodextrin (Captisol®) that were incorporated in a fast-resorbable hydrogel composed of hyaluronic acid grafted with poly-lactic acid (HA-PLA) named DAC® [2]. Moreover, we present assemblies of ZnT4 with a polymeric sulfobutylether-β-cyclodextrin and a nanohybrid of meso-tetrakis(N-methylpyridinium-4-yl)porphine (H_2T4) with silver nanoparticles (AgNPs). AgNPs were produced through the reduction of silver nitrate assisted by a cyclodextrin based polymer bearing citrate functionalities which also acts as stabilizing agent of NPs. Finally, a biodegradable and microporous composite membrane of chitosan (CHT) and porphyrin was developed as a potential patch for the treatment of skin diseases. The composite membrane was developed by incorporating in the dispersion of CHT the Captisol®/H_2T4 photosensitizing nanosystem [3]. All of these biomaterials were fully characterized by spectroscopic and morphological techniques and demonstrated significant photobactericidal activity against a plethora of bacterial strains, including in some case biofilm. Altogether, *in vitro* studies elucidated the photoantimicrobial efficacy of these photosensitizing biomaterials incorporating cyclodextrin/porphyrinoids assemblies.

Acknowledgement: Novagenit (Trento, Italy) and Ligand (San Diego, USA) to provide DAC® and Captisol®, respectively. MUR-PNRR project SAMOTHRACE (ECS:00000022). GM is grateful to Programma Regionale SICILIA FSE+ 2021-2027, Priorità 2, ESO 4.7 (Avviso pubblico n.15/2024) for PhD fellowship.

REFERENCES

1. R. Zagami, A. Rubin Pedrazzo, D. Franco, F. Caldera, L. M. De Plano, M. Trapani, S. Patanè, F. Trotta, A Mazzaglia, Int. J. Pharm. 2023, 637, 122883
2. N. Burduja, N. F. Virzì, G. Nocito, G. Ginestra, M. G. Saita, F. Spitaleri, S. Patanè, A. Nostro, V. Pittalà, A. Mazzaglia, , Int. J. Pharm. 2025, 672, 125283
3. S. Salerno et al, *manuscript in preparation*

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CO_2 Reduction by Cobalt Phthalocyanine: Comparing Aqueous-Phase Batch Reactors and Gas-Fed Flow Electrolyzers

Charles C. L. McCrory[a]

[a]*University of Michigan, Ann Arbor, MI, 48109, USA*

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Converting CO_2 in industrial waste streams into value-added products via the electrochemical CO_2 reduction reaction (CO_2RR) represents a crucial strategy for sustainable manufacturing. Our research has extensively investigated how polymer encapsulation affects cobalt phthalocyanine (CoPc) to tailor the catalyst microenvironment, thereby controlling the rate and selectivity for CO_2 reduction over the competing H_2 evolution reaction. Specifically, we have shown that encapsulating CoPc within a coordinating polyvinylpyridine polymer enhances its activity and selectivity for the CO_2RR in aqueous phosphate solutions. This enhancement is due to the polymer's ability to modify the local coordination environment and facilitate substrate transport to the catalyst's active sites. However, like many in the field of catalyst design and development, our previous work has focused on aqueous-phase batch reactors (e.g., H-cells), where CO_2 is supplied from dissolved CO_2 in aqueous solutions at concentrations below 34 mM. In this presentation, we will examine how polymer effects on catalytic activity for CO_2RR transfer from aqueous-fed batch reactors to more practical gas-fed flow electrolyzers. We will compare the CO_2RR activity of polymer-encapsulated CoPc with various polymers in both aqueous-fed batch reactors and gas-fed flow electrolyzers and discuss which polymer properties influence activity and selectivity in each case. We will explore the mechanistic reasons why CO_2 reduction to CH_3OH by CoPc is feasible in solution-fed batch reactors but remains challenging in single-pass gas-fed flow electrolyzers. Additionally, we will consider design parameters for gas-fed flow electrolyzers that can improve the single-pass conversion efficiency of CO_2 to CH3OH by CoPc. Overall, this presentation will emphasize the importance of considering practical applications throughout all stages of electrocatalyst design

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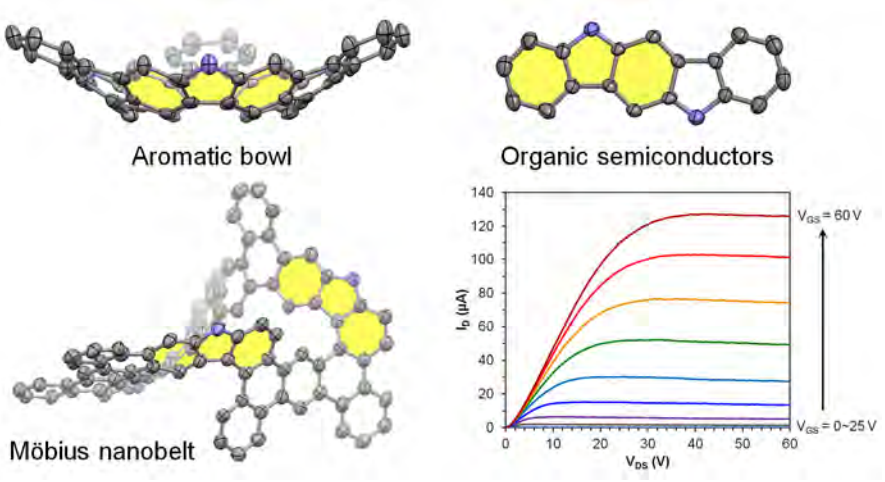
Carbazole-Based Macrocycles and Semiconductors: From Geometric Diversity to Electronic Devices

Qian Miao[a,b,c], Mengna Zhao[a], Han Chen[a], Xin Xie[a], Hushu Ma[a]

[a] *Deparment of Chemistry, The Chinese University of Hong Kong, Hong Kong, China*
[b] *Shanghai-Hong Kong Joint Laboratory in Chemical Synthesis, The Chinese University of Hong Kong, Hong Kong, China*
[c] *State Key Laboratory of Synthetic Chemistry, The Chinese University of Hong Kong, Hong Kong, China*

ORALS

Like pyrrole in porphyrin synthesis, carbazole can serve as a versatile building block for conjugated macrocycles with distinct geometries. The first part of this presentation will highlight the synthesis and structural characterization of carbazole-based macrocycles adopting bowl-shaped [1] and Möbius geometries [2], in contrast to conventional planar analogues. Carbazole derivatives are also powerful scaffolds for organic semiconductors. The second part will focus on p-type and n-type semiconductors [1, 3] built from π-conjugated frameworks incorporating fused carbazole units, with an emphasis on their applications in organic field-effect transistors.



Acknowledgment: This research was supported by the Research Grants Council of Hong Kong (CRF C4001-23G).

REFERENCES

1. Zhao, M.; Pun, S. H.; Gong, Q. Miao, Q. *Angew. Chem. Int. Ed.*, **2021**, *60*, 24124–24130.
2. Chen, H.; Ma, H.; Miao, Q. manuscript in preparation.
3. Zhao, M.; Zhang, B.; Miao, Q. *Angew. Chem. Int. Ed.*, **2020**, 59, 9678–9683

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A Subphthalocyanine-Based Platform for Probing Chirality and Polarity Effects

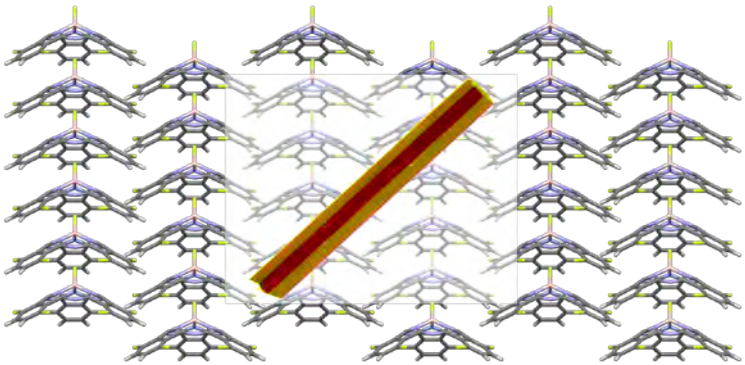
Daigo Miyajima[a]

School of Science and Engineering, The Chinese University of Hong Kong, Shenzhen, China

ORALS

Our recent materials design efforts have focused on chiral bowl-shaped π-conjugated molecules, particularly subphthalocyanine (SubPc), due to its tunable symmetry, well-defined curvature, and capacity to form well-ordered, one-dimensional stacked assemblies.[1,2] We recognized that the C_3-symmetric SubPc framework is uniquely suited to address a fundamental challenge in materials science: how to systematically isolate and study the effects of crystallographic symmetry—such as polarity and chirality—on physical properties, without concurrent changes to core molecular electronic structure.

In this work, we demonstrate precise control over one-dimensional assembly symmetry by designing a series of closely related SubPc derivatives.[3] Through strategic molecular modification, we successfully obtained multiple crystal forms that differ predominantly in their global symmetry—including polar vs. nonpolar and enantiopure vs. racemic alignments—while maintaining nearly identical molecular absorption profiles and frontier orbital characteristics. All structures feature straight columnar stacks, providing a simplified platform to directly correlate symmetry with functional properties. Furthermore, we reveal a general design principle linking molecular shape to preferred packing modes, supported by computational simulations. This family of exceptionally similar yet symmetry-distinct crystals establishes an ideal model system for quantitatively investigating symmetry-dependent phenomena such as chirality-induced spin selectivity and bulk photovoltaic effects.



REFERENCES

1. C. Zhang, K. Nakano, M. Nakamura, F. Araoka, K. Tajima, D. Miyajima, *J. Am. Chem. Soc.*, **142**, 3326–3330, 2020.
2. C. Zhang, Y. Guo, D. He, J. Komiya, G. Watanabe, T. Ogaki, C. Wang, A. Nihonyanagi, H. Inuzuka, H. Gong, Y. Yi, K. Takimiya, D. Hashizume, D. Miyajima, *Angew. Chem. Int. Ed.*, **60**, 3261, 2021.
3. C. Zhang, D. He, B. Dhara, A. Nihonyanagi, H. Inuzuka, E. Hara, S. Sato, K. Adachi, G. Watanabe, D. Hashizume, K. Okuro, D. Miyajima, *Angew. Chem. Int. Ed.*, **2025**, **64**, e202424162.

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Probing active sites outersphere influences in heme and nonheme iron proteins using photolabile exogenous ligand donors at cryogenic temperatures

Pierre Moënne-Loccoz[a]

[a]*Department of Chemical Physiology and Biochemistry,School of Medicine, Oregon Health & Science University, Portland, Oregon 97239, United States*

This oral presentation will first review published studies that utilize photolabiled caged nitric oxide (NO) compounds to produce vibrational characterizations and identifications of transient intermediates in metalloenzymes. Using a photolabile caged NO compound previously characterized by Fujimori and coworkers (1), we obtained resonance Raman and FTIR data demonstrating that release of NO at cryogenic temperatures in presence of oxymyoglobin generates a heme ferric-nitrito complex identical to the one observed using rapid-freeze-quench (RFQ) approach (2,3). The implication of this work is that access to the ferric-superoxo group by NO and isomerization of the ferric-peroxynitrite to ferric-nitrito are optimized steps in the globin active site structure requiring no side chain conformational rearrangements. This conclusion is consistent with the prominent role this reaction plays in the survival of pathogenic microorganisms in infected mammalian macrophages.
Currently, we use this cryogenic approach to probe structural rearrangements in other hemoproteins and nonheme iron proteins and observe spectroscopic signatures of iron-nitrosyl species that, in some instances, suggest we can parse out exogenous ligand binding, endogenous ligand reorganization, and outsphere hydrogen bond partner recruitment processes. These on-going studies will be the main focus of the talk.

REFERENCES

1. Namiki, S., Arai, T., Fujimori, K. (1997) ***J. Am. Chem. Soc. 119***, 3840-3841.
2. Albert, T., Kumar, A., Caranto, J., Moënne-Loccoz, P. (2024) ***J. Inorg. Biochem. 258***, 112633.
3. Yukl, E. T., de Vries, S., Moënne-Loccoz, P. (2009) ***J. Am. Chem. Soc. 131***, 7234-7235.

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Expanding the Toolbox for On-Surface Porphyrin Polymerization *via* Indenyl Coupling

Ana R. Monteiro[a], Jesús Bello-García[a], Alba García-Frutos[b], Aurelio Gallardo[b], Ana Barragán[b], David Écija[b] and Diego Peña[a,c]

[a] *Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS), Departamento de Química Orgánica, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain.*
[b] *IMDEA Nanoscience, Campus de Cantoblanco, C/ Faraday 9, 28049 Madrid, Spain.*
[c] *Oportunius, Galician Innovation Agency (GAIN), 15702 Santiago de Compostela, Spain.*

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Extended π-conjugated frameworks have emerged as key molecular architectures for developing semiconducting materials in optoelectronic applications. Their electronic structures can be tuned through diverse molecular design strategies, including peripheral functionalization, modulation of the conjugation topology, and the incorporation of defects and heteroatoms [1]. Among these approaches, porphyrins (PORs) stand out as verstatile platforms to obtain π-extended systems, owing to their distinctive photophysical features, exceptional chemical and thermal stability, and flexible coordination chemistry with various metal centers [2]. Selective *β*- and *meso*-functionalization of the tetrapyrrolic core, achieved through both in-solution (ISS) and on-surface synthesis (OSS), has granted access to a broad family of fully π-conjugated oligo-porphyrins exhibiting diverse molecular architectures and tunable optoeletronic properties [2-4].

In this work, we have synthesized *meso*-functionalized PORs incorporating dicyclopentaanthracene (DCPA) units (an acene derivative featuring two terminal indene moieties). Through a comprehensive approach combining scanning tunneling microscopy, scanning tunneling spectroscopy, non-contact atomic force microscopy, and density functional theory calculations, we have revealed that these POR-DCPA precursors undergo one-dimensional polymerization on Au(111) surfaces *via* indenyl coupling [5], forming zipper-like chains with efficient π-electron delocalization (Figure 1). In addition, trimeric structures were identified, showing antiaromatic properties. Overall, this work paves the way for tailored π-conjugated hybrids for quantum devices and next-generation organic electronics, offering a successful and unprecedented approach to design porphyrin polymers.

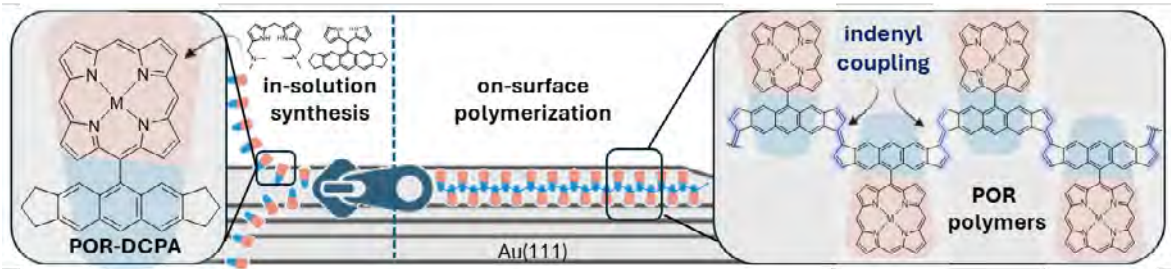


Figure 1. Polymerization of POR-DCPA precursors on Au(111) surface *via* indenyl coupling.

REFERENCES

1. Gu, Y. *et al.*, *J. Am. Chem. Soc.* **2022**, *144*, 11499-11524.
2. Xiang, F. *et al.*, *Nat. Chem.* **2025**, *17*, 1356-1363.
3. Mateo, L. M. *et al.*, *Chem. Sci.* **2021**, *12*, 247-252.
4. Wiengarten, A. *et al.*, *J. Am. Chem. Soc.* **2014**, *136*, 9364-9354.
5. Biswas, K. *et al.*, *Angew. Chem. Int. Ed.* **2025**, e202512575.

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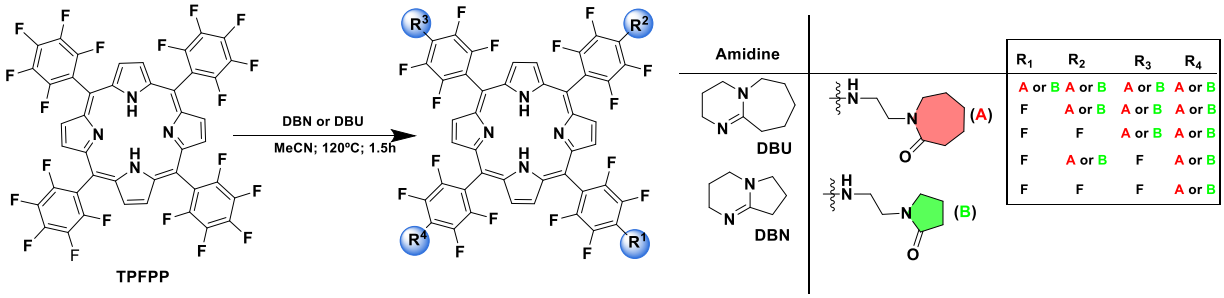
New Porphyrin Functionalized with Azabicyclic Amidines for PDT Applications

Carlos J. P. Monteiro [a], **Ana S. Joaquinito**[a], **Luca Menilli** [b], **Federico Frendo**[b], **Giorgia Miolo** [b], **Maria A. F. Faustino**[a]

[a] LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.
[b] Department of Pharmaceutical and Pharmacological Sciences, University of Padova, Via F. Marzolo 5, 35131 Padova, Italy.

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Photodynamic therapy (PDT) is a clinically established treatment based on the activation of a photosensitizer (PS) by visible light in the presence of dioxygen, leading to the generation of cytotoxic reactive oxygen species (ROS). [1,2]. Compared with conventional anticancer therapies, PDT offers several advantages, including minimal invasiveness, low systemic toxicity, selective cell destruction, good cosmetic outcomes, immune system stimulation, and high tolerability. Despite these benefits, the clinical impact of PDT remains constrained by the limited efficiency of available PSs, highlighting the need for more efficient PSs. Our research group has explored the synthetic versatility of 5,10,15,20-tetrakis(pentafluorophenyl)porphyrin (TPFFP) as a multipurpose scaffold, enabling efficient and selective derivatization via nucleophilic aromatic substitution to generate libraries of biologically relevant photoactive compounds [3]. In this communication, we report new TPFFP derivatives functionalized with azabicyclic amidines, including their structural characterization, photophysical properties, and photodynamic activity against the MDA-MB-468 cell line.



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REFERENCES

1. Hamblin, M.R. *Photochem. Photobiol.* **2020**, 96, 506-516.
2. Mesquita, M.Q.; Dias, C.J.; Neves, M.; Almeida, A.; Faustino, M.A.F. *Molecules* **2018**, 23(10):2424.
3. Costa, J. I. T.; Tomé, A. C.; Neves, M. G. P. M. S.; Cavaleiro, J. A. S. *J. Porphyrins Phthalocyanines* **2011**, 15 (11-12), 1116-1133.

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Anion-Accelerated Photocatalytic Reduction of Carbon Dioxide Using Pyrrole-Based Photosensitizers

Tatsuki Morimoto[a]

[a] *Department of Applied Chemistry, Graduate School of Engineering, Tokyo University of Technology, 1404-1 Katakura, Hachioji, Tokyo 192-0982, Japan.*

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Conversion of carbon dioxide (CO_2) into valuable organic compounds or fuels using sunlight is attracting much interest as a fundamental technology for solving serious problems, such as global warming, energy problems, and so on. Photocatalytic CO_2 reduction can be such a technology, which enables consumption of CO_2 to produce valuable chemicals using solar energy. Many photocatalysts for CO_2 reduction are compose of metal complexes containing rare metals, so that alternative rare-metal-free complexes are required.[1] Herein, we will report new photocatalytic systems adopting photosensitizers comprising pyrrole-based boron complexes, where photocatalytic performance was improved by addition of anion species.

Among rare-metal-free complexes, dipyrrolyldiketone boron complexes were selected, because they can absorb visible light around 500 nm, exhibit fluorescence, and also show anion-binding ability.[2] Photocatalytic CO_2 reduction was conducted using the boron complex as a photosensitizer in combination with a rhenium complex Rebpy$(CO)_3$Br as a catalyst for CO_2 reduction (Figure 1). As a result, turnover number of the CO_2 reduction to CO was about 400 in 9 hours. Moreover, CO formation rate was found to be accelerarted by addition of anion species. For instance, the addition of bromide ion increased the reaction rate constant of CO_2 reduction by a factor of *ca*. 7. According to detailed studies on photophysical and electrochemical properties of the boron complex in the presence/absence of anion species, we found that anion binding of the boron complex induced extended excitation lifetime of the excited state and high reducing power of the one-electron reduced boron complex, which are highly desirable properties as photosensitizers that promote CO_2 reduction. Other photocatalytic systems based on boron complexes with various 1,3-diketone ligands[3] will also be shown.

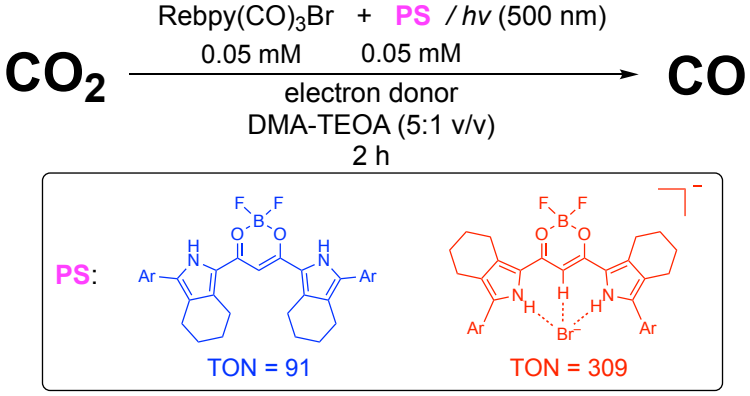


Figure 1. Photocatalytic CO_2 reduction using a pyrrole-based boron complex as a photosensitizer.

REFERENCES

1. Ma, F.; Luo, Z.-M.; Wang, J.-W.; Aramburu-Trošelj, B. M.; Ouyang, G. *Coord. Chem. Rev.* **2024**, *500*, 215529.
2. Maeda, H.; Terasaki, M.; Haketa, Y .; Mihashi, Y .; Kusunose, Y . *Org. Biomol. Chem*. **2008**, *6*, 433-436.
3. Minamikawa, R.; Ishihara, R.; Hatakeyama, K.; Morimoto, T.; Ueno, S., *Chem. Lett.* **2025**, *54*, upaf146

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Modulation of Hydrogen Abstraction Reactivity of a Compound I Model Complex by Axial Ligand π-Donation

Yuma Morimoto

School of Science, Institute of Science Tokyo

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Heme enzymes responsible for the metabolism of lipophilic substrates in vivo utilize an iron(IV)-oxido porphyrin π-cation radical species (Compound I) as the active oxidizing agent. It is known that the axial ligand of Compound I significantly influences its activity in the hydroxylation of alkanes, but the specific properties of the axial ligand contributing to this effect remain unclear. In this study, we systematically investigated the effects of various axial ligands on Compound I model complexes. Fe^{III}(TMP)(L) (TMP = 5,10,15,20-tetramesitylporphyrin dianion) ($\mathbf{1^L}$) were prepared by adding silver salts (Ag**L**, $\mathbf{L}^-$ = NO_3^-, CF_3COO^-, $CHCl_2COO^-$, CH_2ClCOO^-, Cl^-, AcO^-, BzO^-, F^-) to the solution of Fe^{III}(TMP)(Cl) ($\mathbf{1^{Cl}}$). Subsequently, $\mathbf{1^L}$ (28 μM) was oxidized by ozone to produce the corresponding Fe^{IV}(O)($TMP^{+\bullet}$)(L) ($\mathbf{2^L}$), which was used as an oxidant for the cyclohexane hydroxylation (25–400 mM). The pseudo-first-order rate constants for the reaction were determined from the time-dependent changes in the absorption spectra of $\mathbf{2^L}$, and the second-order rate constants (k) were calculated based on the substrate concentration dependence. The value of k varied up to 30-fold depending on the axial ligand. In addition, Fe^{III}(NO)(TMP)(**L**) ($\mathbf{3^L}$) was prepared by coordinating nitric oxide to 1L. The infrared absorption spectra of these complexes showed characteristic peaks attributed to the stretching vibration of NO. The $3CH_3COO$ complex exhibited the lowest wavenumber peak (1858 cm^{-1}), while the $3CF_3COO$ complex displayed the highest (1914 cm^{-1}). These NO stretching frequencies (ν_{N-O}) are considered to reflect the π-donating ability of the axial ligand sensitively.

A plot of the logarithm of the second-order rate constant (ln k) versus ν_{N-O} revealed a good linear correlation (Figure 1), indicating that complexes with more π-donating axial ligands tend to exhibit higher reactivity. These results suggest that axial ligands with higher π-donating ability enhance the electron density and basicity of the oxo ligand, thereby activating the iron-oxo complex.

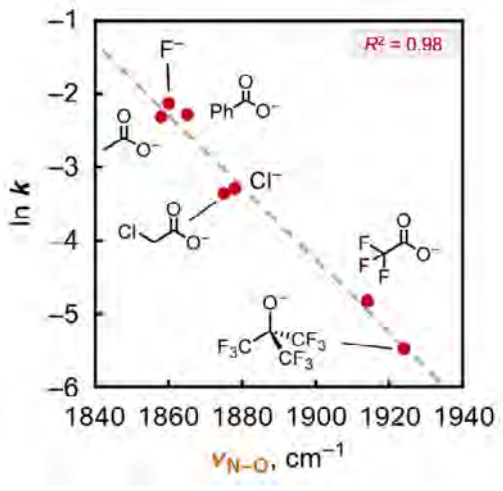


Figure 1. Plot of logalism of k (ln k) against Raman shift of $\mathbf{3^L}$ assignable to ν_{N-O} (L: $(CF_3)_3CO^-$, CF_3COO^-, CH_2ClCOO^-, Cl^-, AcO^-, BzO^-, F^-) assigned to Fe–O bond stretching vibration ($\nu_{Fe=O}$).

REFERENCES

1. Morimoto, Y. ; Shimaoka, Y. ; Ishimizu, Y. ; Fujii, H. ; Itoh, S. *Angew. Chemi. Int. Ed.* **2019**, *58*, 10863–10866.

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Mechanistic Investigations of Carbon Dioxide Reduction by Porphynic MOFs

Amanda J. Morris

Virginia Tech, Blacksburg, USA

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The presented work provides a comprehensive mechanistic picture of the photoinduced processes governing CO_2 reduction in a porphyrinic Zr-based metal–organic framework. By combining spectroscopic experiments with theoretical analysis, we elucidate how light-driven charge-transfer events enable catalytic formate production in MOF-545 under visible light irradiation in the presence of triethanolamine. The study reveals that photoexcitation of the porphyrinic linkers initiates electron transfer processes that ultimately drive CO_2 activation at the Zr_6 nodes. Contrary to commonly proposed models, our results demonstrate that ligand-centered excitation, rather than direct metal-centered charge transfer, plays the dominant role in initiating reactivity. Time-resolved spectroscopic measurements show that photooxidation of the sacrificial donor occurs at the linker sites, generating reactive intermediates that subsequently deliver reducing equivalents to CO_2 bound at the inorganic node. Complementary computational analysis supports a mechanism in which hydride transfer from a transient organic radical species to the Zr-bound CO_2 intermediate constitutes the key bond-forming step. The collaborative effort establishes a unified mechanistic framework that connects photophysics, charge transfer, and catalysis in porphyrinic metal–organic frameworks, highlighting general design principles for promoting multi-electron photochemical transformations in extended materials.

REFERENCES

1. Benseghir, Y.; Sole-Daura, A.; Cairnie, D.R.; Robinson, A.L.; Duguet, M.; Mialane, P.*; Gairola, P.; Gomez-Mingot, M.; Fontecave, M.; Iovan, D.A.; Bonnett, B.; Morris, A.J.*; Dolbecq, A.; Mellot-Draznieks, C.* "Unveiling the Mechanism of the Photocatalytic Reduction of CO_2 to Formate Promoted by Porphrynic Zr-Based Metal-Organic Frameworks." *J. Mater. Chem. A.* 2022, 10, 18103-18115.

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Photodynamic efficacy of cationic porphyrin-triphenylphosphonium conjugates

Nuno M. M. Moura[a], Filipe M. P. Morais[a], Inês Chaves[b], Cátia Vieira[b], M. Graça P. M. S. Neves[a], Adelaide Almeida[b], M. Amparo F. Faustino[a]

[a] *LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal*
[b] *CESAM, Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal*

Modern medical practices depend heavily on antimicrobial treatments, which have played a vital role in increasing global life expectancy.[1] However, the frequent and often unregulated use of antibiotics has led to a rise in drug-resistant microorganims, creating a serious public health challenge. To address this, researchers are actively looking for alternative therapies that can decrease our reliance on traditional pharmacological agents.[2]
Among the most promising alternatives, are porphyrins and related tetrapyrrolic macrocycles which have attracted significant interest due to their versatile (photo)chemical and (photo)physical properties. These compounds are especially well-suited for antimicrobial photodynamic therapy (aPDT), due to their ability to absorb visible light and to produce of reactive oxygen species (ROS) responsible by the eradication of pathogens, while exhibiting high stability, and minimal toxicity in the absence of light.[3,4] Coordination of metal ions within these structures (metalloporphyrins) often results in higher therapeutic efficiency compared to metal-free counterparts, typically by improving ROS generation and/or microbial cells interaction.[5]
In this comunication, the effect of phosphonium units, on the photochemical and photophysical properties of three free-base cationic porphyrin-triphenylphosphonium conjugates and of their corresponding metal complexes is discussed. Their photodynamic activity against two distinct bacterial models: the Gram-positive, methicillin-resistant *Staphylococcus aureus* (MRSA) and the Gram-negative *Escherichia coli* is also analized, showing how the triphenylphosphonium units and the metal ions modulates the photodynamic performance.[5,6]

Funding/Acknowledgements: This research work received financial support from the University of Aveiro and FCT/MCTES to support UID/50006/2023 - Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos research unit. NMM Moura gratefully acknowledges FCT for an Assistant Research Position (2023.06495.CEECIND).

REFERENCES

1. Vieira, C., Gomes, A.T.P.C., Mesquita, M.Q., Moura, N.M.M., Neves, M.G.P.M.S., Faustino, M. A. F., Almeida, A. *Front. Microbiol.* **2018**, *9*, 1–16.
2. Hobson, C., Chan, A.N., Wright, G.D.: The antibiotic resistome: a guide for the discovery of natural products as antimicrobial agents, *Chem. Rev.* **2021**, *121*, 3464–3494.
3. Mesquita, M., Dias, C.J., Neves, M.G.P.M.S., Almeida, A., Faustino, M. A. F. Revisiting current photoactive materials for antimicrobial photodynamic therapy, *Molecules* **2018**, *23*, 2424.
4. Akbar, A., Khan, S., Chatterjee, T., Ghosh, M. Unleashing the power of porphyrin photosensitizers: illuminating breakthroughs in photodynamic therapy, *J. Photochem. Photobiol. B Biol.* **2023**, *248*, 112796.
5. Chaves, I., Morais, F.M.P., Vieira, C., Bartolomeu, M., Gomes, A.T.P.C., Faustino, M. A. F., Neves, M.G.P.M.S., Almeida, Moura, N.M.M. The impact of metal ions on the photo-antibacterial efficiency of metalloporphyrins with triphenylphosphonium units, *Inorg. Chem. Commun.* **2025**, *178*, 114426.
6. Chaves, I., Morais, F.M.P., Vieira, C., Bartolomeu, M., Gomes, A.T.P.C., Faustino, M. A. F., Neves, M.G.P.M.S., Almeida, Moura, N.M.M. Can porphyrin−triphenylphosphonium conjugates enhance the photosensitizer performance toward bacterial strains?, *ACS Appl. Bio Mater.* **2024**, *7*, 5541-5552.

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Remarkable Isomeric Effects on Near-Infrared Absorption and Aromaticity of a Core-Modified Phthalocyanine Incorporating Two Phenolic Groups

Atsuya Muranaka[a,b], **Yu Hatakenaka**[a,b], **Naoyuki Toriumi**[b], **Hiroyuki Koshino**[a], **Masanobu Uchiyama**[a,b]

[a]*Molecular Structure Characterization Unit, RIKEN CSRS, Wako-shi, Saitama 351-0198, Japan*
[b]*Graduate School of Pharmaceutical Sciences, The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*

ORALS

Near-infrared (NIR) absorbing organic compounds have attracted considerable attention over the years since they have various potential applications. Among these, porphyrin-related compounds that can switch their NIR absorption in response to external stimuli are of particular interest not only due to their unique and distinctive optical properties, but also due to their macrocyclic aromaticity. Our research group has previously developed a core modified phthalocyanine, tetrahydroxydicarbahemiporphyrazine (**1**), two-electron oxidation of which leads to the 18π-electron quinoidal form that has an intense NIR absorption peaked at around 850 nm (Figure 1) [1]. During our reserach on switchable NIR-absorbing porphyrinoids, we became interested in the substituent effects of the core modified phthalocyanine on the optical and switching properties, as the number of hydroxy groups is responsible for the NIR-absorption wavelength for related benziphthalocyanines [2]. Herein we report synthesis and properties of the *anti*- and *syn*-isomers of dihydroxydicarbahemiporphyrazine (**2**$_{anti}$, **2**$_{syn}$). Both isomers were readily oxidized by oxidants, and the resulting two-electron oxidized forms exhibited remarkable isomeric effects. The oxidized form of **2**$_{anti}$ exhibited distinct NIR absorption over 900 nm in $CHCl_3$, whereas weak and broad bands were observed in the 500-1000 nm region for the corresponding *syn*-isomer. The ^{1}H NMR spectra indicated that the presence of diatropic ring current effect in the oxidized form of **2**$_{anti}$. No such ring current effect was observed for the *syn*-isomer. Density functional theory calculations suggested that a nonaromatic asymmetric tautomer plays a pivotal role in the optical properties and aromaticity in the two-electron oxidized form of **2**$_{syn}$.

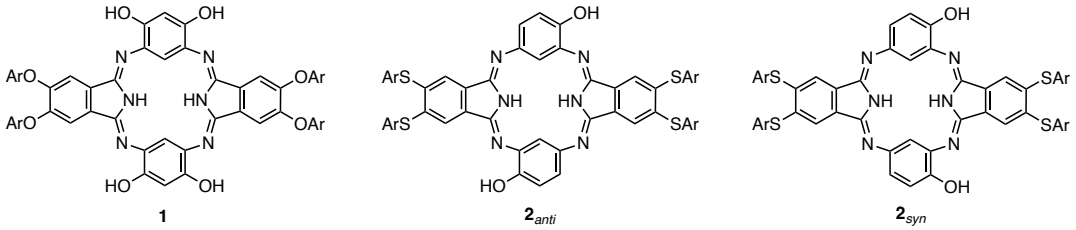


Figure 1. Chemical structures of tetrahydroxydicarbahemiporphyrazine (**1**) and the *anti*- and *syn*-isomers of dihydroxydicarbahemiporphyrazine (**2**$_{anti}$, **2**$_{syn}$). Ar = 2,6-dimethylphenyl.

REFERENCES

1. Muranaka, A.; Ohira, S.; Hashizume, D.; Koshino, H.; Kyotani, F.; Hirayama, M.; Uchiyama, M. *J. Am. Chem. Soc*. **2012**, *134*, 190-193.
2. Toriumi, N.; Asano, N.; Ikeno, T.; Muranaka, A.; Hanaoka, K.; Urano, Y.; Uchiyama, M. *Angew. Chem. Int. Ed.* **2019**, *58*, 7788-7791.

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Photorelease of Reactive Carbon Species from Organorhodium Phthalocyanine Complexes

Kei Murata[a,b,c], Yuki Saibe[a], Mayu Uchida[a], Mizuki Aono[a], Ryuji Misawa[a], Yoshiho Ikeuchi[a], Kazuyuki Ishii[a]

[a]*Institute of Industrial Science, The University of Tokyo*
[b]*RIKEN Center for Sustainable Resource Science,* [c]*RIKEN Pioneering Research Institute*

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Photodynamic therapy has attracted considerable attention as a minimally invasive cancer treatment based on tumor-selective cell attack.[1] However, because this therapy relies on the photochemical generation of reactive oxygen species by photosensitizers, the mechanism of cell death induction is limited, and the therapeutic efficacy is low in hypoxic regions within tumors, where oxygen concentrations are low. To address these issues, in this study, we have developed the red light uncaging reactions of the organorhodium phthalocyanine complexes which generate reactive carbon species such as alkyl radicals and aldehydes (Figure 1).[2] This hybrid system integrating PDT with photouncaging reactions is expected to enable effective tumor cell treatment under diverse oxygen environments.[3]

Complexes bearing simple alkyl ligands were found to release alkyl radicals from their axial ligands via stepwise two-photon excitation using a nanosecond pulsed laser of red light, whereas complexes bearing benzyl or allyl ligands underwent similar reactions through single-photon excitation of a continuous wave of red light. These alkyl radicals were readily converted into terminal aldehydes in the presence of oxygen, a process that proceeded even under hypoxic conditions owing to the involvement of the rhodium center. Based on this principle, several apoptosis inducers possessing a terminal aldehyde as the active group were successfully released by red light irradiation. The complexes were introduced into HeLa cells via encapsulation in phospholipid bilayers. Phototoxicity experiments demonstrated that the complexes exhibit photodynamic effects across a wide range of oxygen conditions.

The details on the photophysical and photochemical properties of the complexes will be discussed in the presentation.

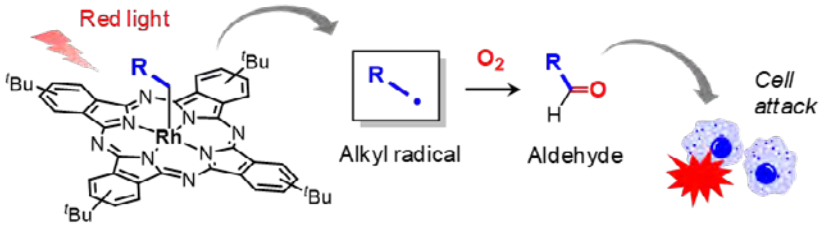


Figure 1. Photouncaging reaction of the rhodium phthalocyanine complexes.

REFERENCES

1. P.-C. Lo, M. S. Rodriguez-Morgade, R. K. Pandey, D. K. P. Ng, T. Torres, F. Dumoulin, *Chem. Soc. Rev.*, **2020**, *49*, 1041–1056.
2. K. Murata, Y. Saibe, M. Uchida, M. Aono, R. Misawa, Y. Ikeuchi, K. Ishii, *Chem. Commun.*, **2022**, *58*, 11280–11283.
3. E. D. Anderson, A. P. Gorka, M. J. Schnermann, *Nat. Commun.*, **2016**, *7*, 13378.

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The Chiral Induced Spin Selectivity- Why is it so special?

Ron Naaman

Weizmann Institute, Department of Chemical and Biological Science, Rehovot 76100, Israel

The Chiral Induced Spin Selectivity (CISS) effect was first observed more than 25 years ago. Despite numerous experimental verifications across chemistry, physics, and biology, many feel that the underlying mechanism remains poorly understood. This talk will address the question: what makes CISS fundamentally different from conventional electron transport? and will provide new insights into its mechanism. It will be demonstrated how chirality necessitates a fresh perspective on electron transfer and present experimental evidence for the key parameters that enable the CISS effect, challenging our conventional understanding of electronic transport phenomena

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Gas-Phase Synthesis of Porphyrin-based Donor-Acceptor Covalent Organic Framework Thin Films: Electrocatalysts for OER and ORR

Deepak Bansal, Nicolas D. Boscher and Amr A. Nada*

Luxembourg Institute of Science and Technology, Advanced Plasma and Vapor Deposition Processes, L-4362, Esch-sur-Alzette, Luxembourg.

Bifunctional electrocatalysts for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) are central to the development of fuel cells and metal–air batteries, yet their performances are often limited by poor electrical connectivity and poorly defined active sites. These limitations mainly arise from the synthesis strategies commonly employed, which inherently lead to structural and electronic heterogeneity, resulting in non-uniform active sites and inefficient charge-transport pathways. Here, we report the simultaneous vapor-phase synthesis and deposition of porphyrin-based donor-acceptor covalent organic frameworks (COFs) via solid–vapor Schiff-base condensation.

The resulting porphyrin–based COF thin films are homogeneous, electrically conductive, and feature well-defined active sites and a favourable band alignment for oxygen electrocatalysis [1]. Electrochemical measurements in alkaline media demonstrate bifunctional ORR/OER activity, with ORR half-wave potentials approaching 0.35 V *vs.* RHE and diffusion-limited current densities on the order of -300 $\mu A \cdot cm^{-2}$, comparable to state-of-the-art porphyrin-based COFs reported in the literature [1, 2]. For OER, the vapor-grown thin films reach 700 $\mu A \cdot cm^{-2}$ at overpotentials below 400 mV, placing them among the most active non-pyrolyzed porphyrin-based covalent organic frameworks.

Compared to solution-grown or post-pyrolyzed COFs, the vapor-phase route yields superior charge transport and interfacial coupling, which directly translate into improved reaction kinetics and reduced bifunctional potential gaps (ΔE). These results highlight the unique advantages of gas-phase synthesis for constructing electrocatalyst thin films based on extended conjugated organic frameworks and establish the vapor-phase route as a promising and scalable method for the engineering of such films.

REFERENCES

1. Shao, P., et al., Journal of the American Chemical Society, 2025. **147**(10): p. 8769-8777.
2. Liao, L., et al., Inorganic Chemistry Frontiers, 2025. **12**(5): p. 1881-1889.

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Nitric Oxide Binding to *meso*-Tetraphenylporphyrin Fe(II/III) Complexes Encapsulated in the Cyclodextrin Nanocavities in Aqueous Solution

Atsuki Nakagami[a], Masahito Kodera[b], Hiroaki Kitagishi[b]

[a]*Department of Applied Chemistry, Graduate School of Engineering, The University of Osaka, Japan.*
[b]*Dept. of Molecular Chemistry & Biochemistry, Faculty of Science and Engineering, Doshisha University, Japan.*

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Nitric oxide (NO) strongly binds to heme in soluble guanylate cyclase (sGC), thereby mediating several biological functions, including vasodilation in the mammalian body. While a large number of studies have been conducted to elucidate the heme−NO interaction, we investigated it using a unique water-soluble synthetic model, hemoCD. HemoCD consists of *meso*-tetraphenylporphinatoiron tetrasulfonate (FeTPPS) that is encapsulated by per-*O*-methylated β-cyclodextrin dimers linked by nitrogenous ligands [1]. In this work, UV−vis, resonance Raman, and EPR spectroscopies revealed the formation of both ferric and ferrous nitrosyl complexes of hemoCD in water [2]. We used two types of hemoCD, hemoCD-P with a pyridine linker and hemoCD-I with an imidazole linker, and both hemoCDs show comparable affinities for NO to those of native hemoglobin, as well as for other small gaseous molecules such as O_2, CO, HCN, and H_2S. But the different reactivity between hemoCD-P and -I against reductive nitrosylation was clearly observed because of their structural difference. Due to the reductive nitrosylation, ferric nitrosyl hemoCD complexes were observed in acidic glycine buffer solution. However, N_2 gas was unexpectedly generated during the experiment [3]. After careful investigation, a N−N bond formation between NO and glycine on hemoCD was shown by both experimental and theoretical studies. N_2 gas was finally produced from the diazo intermediate by S_N2 reaction with water. Although this reaction proceeds under specific conditions, we believe these models would offer new possibilities for considering the heme−NO interaction.

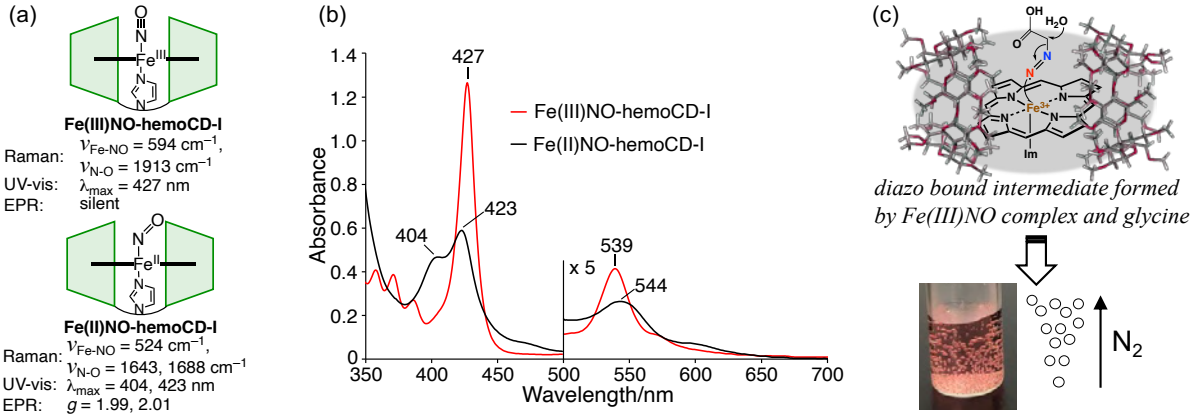


Fig. (a) Ferric and ferrous nitrosyl complexes of hemoCD-I with spectroscopic data. (b) UV−vis spectra of nitrosyl hemoCD-I complexes. (c) N_2 gas generation from ferric nitrosyl hemoCD complex with glycine in acidic glycine buffer solution.

REFERENCES

1. Kitagishi H, Kano K, *Chem. Commun*. 2021; **57**: 148−173.
2. Nakagami A, Tosha T, Horitani M, Oohora K, Hayashi T, Sato W, Kubo M, Kodera M, Kitagishi H, *Inorg. Chem*. 2025; **64**: 13973−13985.
3. Nakagami A, Shiota Y, Fujikawa K, Kodera M, Kitagishi H, *J. Am. Chem. Soc*. 2025; **147**: 47898−47903.

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π–Gel electrets toward deformable vibration sensors

Takashi Nakanishi[a,b]

[a]*Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Tsukuba, Japan*
[b]*Division of Soft Matter, Graduate School of Life Science, Hokkaido University, Sapporo, Japan*

The development of optoelectronically active soft materials has become increasingly important for applications in soft (bio)electronics. Room-temperature, solvent-free alkyl–π liquids, obtained by functionalizing π–conjugated units with bulky, flexible branched alkyl chains, are promising new functional soft materials. The π–conjugated units responsible for optoelectronic functions are protected by insulating and high-entropy branched alkyl chains, enabling these functions to be exhibited even in the bulk liquid state at room temperature. Various optically functional liquids have been developed, including those capable of emitting light [1] and generating singlet oxygen [2]. Meanwhile, we have successfully developed π–liquid electrets, including porphyrins [3] and C_{60} fullerenes [4] as the functional π–unit, that stably retain charges at the surface and within the interior of alkyl–π liquids, as well as freely deformable electret devices, particularly for use in vibration sensors. In this presentation, we discuss the creation of π–gels from an alkyl–pyrene liquid [5] (Fig. 1), their electretization, and the application of freely deformable, weak-vibration sensors based on π–gel electret devices [6].

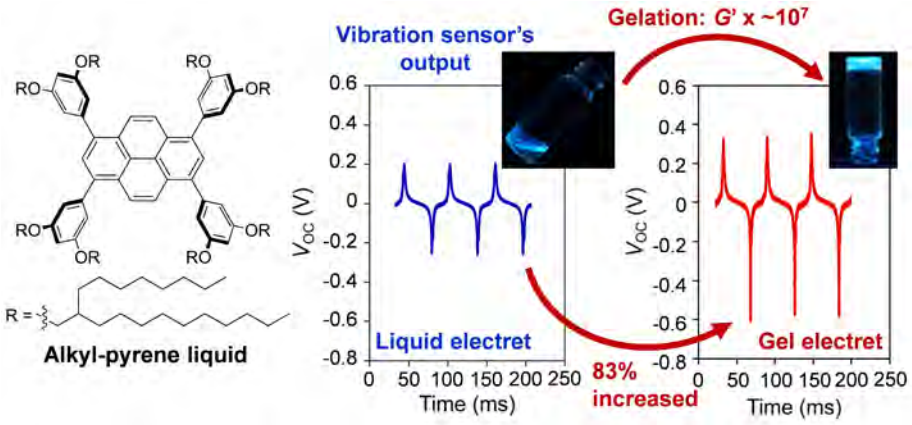


Fig. 1. Alkyl-pyrene liquid and gel electrets and their vibration sensor's outputs.

REFERENCES

1. Z. Guo, C. Pan, A. Shinohara, T. Nakanishi, *Sci. Technol. Adv. Mater.*, **26**, 2515007 (2025).
2. R. K. Gupta, T. Nakanishi, D. T. Payne, *Chem. Eur. J.*, **31**, e202500739 (2025)
3. A. Ghosh, T. Nakanishi, and others, *Nat. Commun.*, **10**, 4210 (2019).
4. R. K. Gupta, M. Yoshida, A. Saeki, Z. Guo, T. Nakanishi, *Mater. Horiz.*, **10**, 3458 (2023).
5. A. Tateyama, K. Nagura, M. Yamanaka, T. Nakanishi, *Angew. Chem., Int. Ed.*, **63**, e202402874 (2024).
6. D. Nishioka, A. Tateyama, H. Kitano, T. Nakanishi, K. Terabe, T. Tsuchiya, submitted.

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Catalytic Activity of a Dinuclear Iron Complex Bearing a Doubly N-Confused Hexaphyrin toward Photocatalytic CO_2 Reduction and Water Oxidation

Takashi Nakazono[a]

[a]*Research Center for Artificial Photosynthesis (ReCAP), Osaka Metropolitan University, 3-3-138 Sugimoto, Sumiyoshi, Osaka 558-8585, Japan*

ORALS

Artificial photosynthesis, which integrates CO_2 reduction and water oxidation driven by solar energy, is a promising strategy for addressing global warming and fossil fuel depletion. Redox-active macrocyclic ligands offer a versatile platform for multielectron accumulation in molecular catalysis. Herein, we report a dinuclear iron complex with a doubly N-confused hexaphyrin (Fe_2DNCH; Figure 1) as an efficient molecular catalyst for photochemical CO_2 reduction. Under visible-light irradiation in an acetonitrile/water mixed solvent using $[Ru(dmb)_3]^{2+}$ (dmb; 4,4'-Dimethyl-2,2'-bipyridyl) as a photosensitizer and 1,3-dimethyl-2-aryl-2,3-dihydro-1H-benzo[d]imidazole (BIH) as a sacrificial reductant, Fe_2DNCH selectively catalyzed the two-electron reduction of CO_2 to CO with high efficiency. A maximum turnover number of 400 and a CO selectivity of 99% were achieved.[1]

Electrochemical and spectroelectrochemical studies revealed multiple reversible redox processes, indicating that the DNCH ligand serves as a redox-active center capable of multielectron storage. The five-electron-reduced species was identified as the catalytically active form for CO_2 reduction, highlighting the cooperative action of the dinuclear iron centers and the π-conjugated DNCH ligand.

Notably, Fe_2DNCH also exhibited exceptionally high activity for photocatalytic water oxidation in the presence of $[Ru(bpy)_3]^{2+}$ and peroxydisulfate as a sacrificial oxidant. The dinuclear iron complex achieved a turnover frequency of 8.7 s^{-1} and a turnover number of 2,730, significantly outperforming the heterobimetallic FeZn analogue. These results demonstrate that Fe_2DNCH functions as a bifunctional molecular catalyst capable of promoting both photochemical CO_2 reduction and water oxidation.

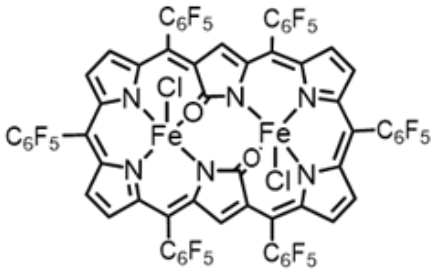


Figure 1. Molecular Staracture of Fe_2DNCH

REFERENCES

1. T. Nakazono, D. Sugawara, T. Ito, Y. Yamada, T. Wada, *Chem. Lett.* **2023**, *52*, 481–484.

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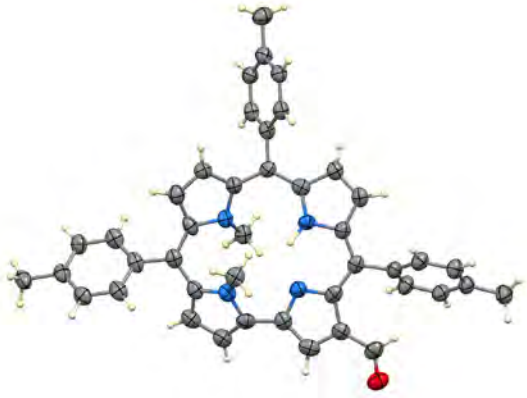


N,N-dimethylcorroles: functionalizations and applications

Sara Nardis [a], Alessia Fata,[a] Francesco Pizzoli,[a] Greta Imbesi,[a] Greta Petrella,[a] Daniel O. Cicero,[a] Frank R. Fronczek,[b] Kevin M. Smith,[b] and Roberto Paolesse[a]

[a] *Department of Chemical Sciences and Technologies, University of Rome Tor Vergata, via della Ricerca Scientifica, 00133 Rome, Italy*
[b] *Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803, USA*

The chemistry of N-alkylated corroles [1-4] remains largely unexplored, despite its significant potential as a powerful strategy for fine-tuning the structural, electronic, and optical properties of this class of porphyrinoids. In this contribution, we present a systematic investigation of the β-formylation of N(21),N(22)-dimethyl-5,10,15-tritolylcorrole, highlighting how a careful modulation of the functionalization sequence allows selective access to different regioisomeric products. Remarkably, the resulting β-formyl-N(21),N(22)-dimethyl-5,10,15-tritolylcorrole exhibits an unprecedented reactivity toward acetone under basic conditions, leading to the efficient formation of a conjugated vinyl ketone derivative in good yields [5]. The newly obtained corrole derivatives display distinctive and tunable optical features, underscoring their potential relevance for future applications in areas such as sensing or advanced functional materials.



REFERENCES

[1] Koszarna, B.; Gryko, D.T. One-pot synthesis of meso-tris-aryl-substituted N-21-methyl- and N-21-benzyl-corroles.Tetrah. Lett. 2006, 47, 6205–6207.
[2] Gross, Z.; Galili N. N-Substituted Corroles: A Novel Class of Chiral Ligands. *Angew Chem Int Ed Engl.* 1999, 38,16, 2366-2369.
[3] Pizzoli, F.; Mita, A.; Caroleo, F.; Nardis, S.; Calice, U.; Caporale, M.; Belviso, S.; Superchi, S.; Marconi, A.; Calvaresi, M.; Capolungo, C.; Prodi, L.; Smith, K. M.; Fronczek F. R.; Paolesse, R. Palladium Complexes of N-Methylcorroles. Chem. Eur. J. 2023, 29.
[4] Pizzoli, F.; Nardis, S.; Fata, A.; Marsotto, M.; Petrella, G.; Fronczek, F.R.; Smith, K.M.; Paolesse, R. N-Alkylcorroles. J. Porphyrins Phthalocyanines 2024, 28 (06), 358-369.
[5] Nardis, S.; Fata, A. ; Pizzoli, F.; Imbesi, G. ; Petrella, G. ; Cicero, D.O. ; Fronczek, F.R. ; Smith, K.M. ; Paolesse, R. ACS Omega 2025, 10, 40, 47129–47140.

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Triply-Fused Porphyrin-Nanographene Conjugates with NIR Absorption and Related Nanographenes with Zigzag Edges

Akimitsu Narita[a,b]

[a]*Okinawa Institute of Science and Technology Graduate University, Okinawa 904-0495, Japan*
[b]*Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany*

ORALS

Large polycyclic aromatic hydrocarbons (PAHs) have been extensively studied as nanographenes, demonstrating intriguing structure-dependent optoelectronics, photophysical, and magnetic properties. Especially, nanographenes with zigzag edges exhibit promising optical properties, e.g., red-shifted and strong fluorescence and stimulated emission. We have previously demonstrated that zigzag-edged nanographenes can be triply fused to a porphyrin, affording planar Ni(II) porphyrin-nanographene conjugates with one or two fused nanographenes, showing near infrared (NIR) absorption up to 1000 and 1400 nm, respectively [1]. Interestingly, Ni(II) porphyrin fused with one nanographene displayed NIR emission at 970 nm with a vibronic peak at 1103 nm, along with stimulated emission at corresponding wavelengths [2]. Moreover, the porphyrin fused with two nanographenes could serve as phototherenostic agents in the NIR-II (1000–1700 nm) window, enabling phoacoustic imaging (PAI)-guided photothermal therapy (PTT) of cancer under 1064-nm laser irradiation [3]. We have also been exploring unprecedented nanographenes with unique structures and properties, featuring zigzag edges where porphyrin can potentially be triply fused. In particular, we have synthesizsed a series of nanographenes having zigzag and fjord edges, resulting in structures with planar core and helical nonplanar peripheries. For example, dibenzo[*a*,*m*]dinaphtho[3,2,1-*ef*:1',2',3'-*hi*]coronene (DBDNC) with one fjord edge demonstrated emission maximum at 643 nm with vibronic signals at 698 and 772 nm and photoluminescence quantum yield (PLQY) of 53% [4]. After encapsulation with amphiphilic polymers into water-dispersible nanoparticles, DBDNC could be applied as NIR-emmisive neuronal tracer with high photostability and biocompatibility for studying the axonal transport in neurons [5]. We have also achieved more extended nanographenes with two fjord edges, demonstrating NIR emission in the range of 800–1000 nm as well as NIR chiroptical resopnses up to 850 nm [6].

REFERENCES

1. Chen, Q.; Brambilla, L.; Daukiya, L.; Mali, K. S.; De Feyter, S.; Tommasini, M.; Müllen, K.; Narita, A. *Angew. Chem. Int. Ed*. **2018**, *57*, 11233–11237.
2. Garcia-Orrit, S.; Vega-Mayoral, V.; Chen, Q.; Serra, G.; Guizzardi, M.; Romano, V.; Dal Conte, S.; Cerullo, G.; Di Mario, L.; Kot, M.; Loi, M. A.; Narita, A.; Müllen, K.; Tommasini, M.; Cabanillas-González, J. *J. Phys. Chem. Lett*. **2024**, *15*, 10366–10374.
3. Zhao, H.; Wang, Y.; Chen, Q.; Liu, Y.; Gao, Y.; Müllen, K.; Li, S.; Narita, A. *Adv. Sci*. **2024**, *11*, 2309131.
4. Xu, X.; Serra, G.; Villa, A.; Muñoz-Mármol, R.; Vasylevskyi, S.; Gadea, M.; Lucotti, A.; Lin, Z.; Boj, P. G.; Kabe, R.; Tommasini, M.; Díaz-García, M. Á.; Scotognella, F.; Paternò, G. M.; Narita, A. *Chem. Sci*. **2022**, *13*, 13040–13045.
5. Zhao, H.; Guillaud, L.; Emily, M. F.; Xu, X.; Moshniaha, L.; Hanayama, H.; Kabe, R.; Terenzio, M.; Narita, *ACS Nano* **2024**, *18*, 34730-34740.
6. Xu, X.; Yang, Q.; Zhao, H.; Vasylevskyi, S.; Bonn, M.; Liu, X.; Narita, A. *Adv. Funct. Mater*. **2024**, *34*, 2308110.

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Elucidation of the Electronic Structure of Modified Porphyrins and Their Analogues Using Experimental and Theoretical Methods

Victor N. Nemykin

Department of Chemistry, University of Tennessee – Knoxville, Knoxville, TN USA vnemykin@utk.edu

The electronic structure of the core-modified porphyrins (i.e., chlorin-, isobacteriochlorin-, and bacteriochlorin-type as well as corrololes and N-confused porphyrins) will be discussed via a prism of the experimental (i.e., UV-Vis-NIR and Magnetic Circular Dichroism, MCD) and theoretical (Density Functional Theory, DFT, and Time-Dependent DFT, TDDFT) methods. General trends of the ΔHOMO and ΔLUMO (ΔHOMO is the energy difference between the Gouterman's "a_{1u}"- and "a_{2u}"-type MOs, and ΔLUMO is the energy difference between the Gouterman's "$e_g(x)$"- and "$e_g(y)$"-type MOs) in modified porphyrins will be discussed.

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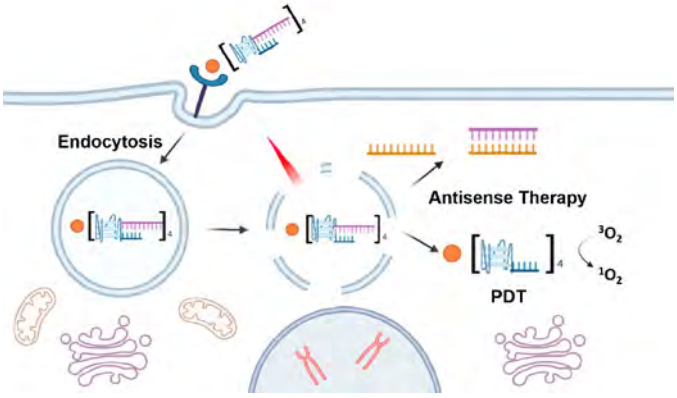
Carrying Photosensitizers and Antisense Oligonucleotides with a G-Quadruplex Platform for Synergistic Photodynamic and Antisense Therapy

Ka-Hin Chan, Dick Yan Tam, and Dennis K. P. Ng*

Department of Chemistry, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China

ORALS

Combination therapy has been proven as an effective strategy for cancer treatment [1]. To this end, we have developed a series of self-assembled nucleic acid-based complexes for synergistic photodynamic and antisense therapy [2]. They contain a nucleolin-targeting G-quadruplex platform, a partially hybridized antisense oligonucleotide (ASO) that can inhibit the anti-apoptotic protein B cell lymphoma-xL (Bcl-xL) protein or the signal transducer and activator of transcription 3 (STAT3) protein, as well as a zinc(II) phthalocyanine (ZnPc)-based photosensitizer held by noncovalent interactions. The complexation of the three components has been optimized by spectroscopic titration. Through a series of in vitro experiments, we have demonstrated that these DNA complexes can be internalized selectively to nucleolin-overexpressed cancer cells through receptor-mediated endocytosis and are localized in the lysosomes. Upon light irradiation, the photosensitization of ZnPc triggers the formation of reactive oxygen species for cell killing and promotes the lysosomal escape of the ASOs for antisense therapy. The combined therapeutic effect and downregulation of crucial downstream targets have been studied systematically. The results will be presented and discussed in this presenation.



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REFERENCES

1. Mokhtari, R. B.; Homayouni, T. S.; Baluch, N.; Morgatskaya, E.; Kumar, S.; Das, B.; Yegar, H. Combination therapy in combating cancer. *Oncotarget* **2017**, *8*, 39022-38043.
2. Tam, D. Y.; Lau, W. K. M.; Limanto, Y. T.; Ng, D. K. P. Light-Promoted Lysosomal Escape of a Phthalocyanine and Antisense Oligonucleotide-Complexed G-Quadruplex for Dual Photodynamic and Antisense Therapy. *ACS Pharmacol. Transl. Sci.*, **2024**, *7*, 3216-3227.

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Dialing In Reactivity and Selectivity of CO_2 Reduction through Second-Sphere Design

Eva M. Nichols[a]

[a]*University of British Columbia*

The activity and selectivity of molecular electrocatalysts are often governed not only by the primary metal coordination environment, but also by local secondary interactions that control proton and substrate delivery. Inspired by enzymatic active sites, our group has focused on iron porphyrins as a well-defined model system to probe how second coordination sphere (SCS) acids influence electrocatalytic CO_2 reduction. Incorporation of appropriately positioned acidic SCS groups generally enhances rates for reactions involving proton-coupled electron transfer, most notably for the two-electron, two-proton reduction of CO_2 to CO.

We recently reported a family of electronically identical iron tetraphenylporphyrin catalysts bearing amide-based SCS proton donors of systematically varied acidity.[1] Linear free-energy relationships revealed that CO_2 reduction kinetics depend not only on the pK_a of the SCS acid, but also on the identity of the bulk proton source. Building on this precedent, the present talk will focus on how selectivity for CO_2 reduction versus competing proton reduction is governed by both the acidity and positioning of the SCS group. We show that optimal SCS positioning suppresses indiscriminate protonation pathways that lead to hydrogen evolution or porphyrin decomposition, while promoting productive CO_2 activation.[2] We report an experimental mechanistic analysis that highlights specific roles for the acidic SCS group in modulating thermodynamic and kinetic parameters, ultimately explaining the observed selectivity trends. Collectively, these results demonstrate how rational second coordination sphere design enables iron porphyrins to achieve high selectivity under conditions that would otherwise favor unproductive proton reduction, providing general design principles for selective molecular CO_2 electrocatalysis.

[1] Teindl, K.; Patrick, B.O.; Nichols, E.M. *J. Am. Chem. Soc.* **2023**, 145, 31, 17176–17186.
[2] Teindl, K.; Reid, J.P.; Nichols, E.M. *Chem. Sci.*, **2025**, 16, 19226–19234.

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Polymer-photosensitizer conjugates for tumor-targeted photodynamic therapy

Takahiro Nomoto[a]

[a]*Graduate School of Arts and Sciences, TheUniversity of Tokyo*

ORALS

Photodynamic therapy (PDT) is a promising, minimally invasive modality for cancer treatment; however, its clinical efficacy is often compromised by the limited tumor selectivity of photosensitizers. To overcome this challenge, we have developed functional polymeric nanomedicines designed to actively recognize tumor-specific markers or respond to the unique tumor microenvironment.

In the early phase of our research, we focused on active targeting of $\alpha_v\beta_3$ integrin, which is overexpressed in tumor-associated neovasculature. We synthesized hydrophilic block copolymers conjugated with a photosensitizer (IRDye 700DX) and multiple cyclic RGD (cRGD) peptides [1]. Our results demonstrated that the multivalent display of cRGD peptides significantly enhanced accumulation in tumor blood vessels, leading to potent antitumor effects upon irradiation.

In parallel, we explored stimuli-responsive strategies by developing a pH-sensitive polymer based on poly(*N*-isopropylacrylamide) (PNIPAAm) [2]. By incorporating an acid-labile hydrophilic moiety, we achieved a sharp, isothermal hydrophilic-to-hydrophobic phase transition in the mildly acidic tumor microenvironment (pH < 6.8). This phase transition promoted cellular interaction and enhanced tumor accumulation compared to conventional non-responsive polymers.

Recently, our focus has shifted to targeting the L-type amino acid transporter 1 (LAT1/SLC7A5) for intracellular drug delivery, as LAT1 is highly upregulated in various cancers to support rapid proliferation [3]. We first identified that polymers modified with methionine (Met) exhibited superior LAT1-selective uptake and tumor accumulation compared to cysteine-modified analogs, highlighting the potential of Met as an effective ligand [4].

Furthermore, to optimize such interaction, we investigated the structural impact of spacer length using tyrosine-modified polymers. We discovered that an appropriately long spacer (e.g., triethylene glycol) is critical for the ligand to access the deep substrate-binding pocket of LAT1 (~20 Å from the surface), thereby enhancing targeting efficiency and therapeutic efficacy [5].

This talk will summarize these design strategies ranging from multivalency and environmental responsiveness to precise structural engineering of ligands for the development of drug delivery systems for PDT.

REFERENCES

1. Dou, X. et al. Effect of multiple cyclic RGD peptides on tumor accumulation and intratumoral distribution of IRDye 700DX-conjugated polymers. Sci. Rep. 8, 8126 (2018).
2. Muttaqien, S. E. et al. Photodynamic therapy using LCST polymers exerting pH-responsive isothermal phase transition. J. Control. Release 328, 608-616 (2020).
3. Nomoto, T. et al. Poly(vinyl alcohol) boosting therapeutic potential of *p*-boronophenylalanine in neutron capture therapy by modulating metabolism. Sci. Adv. 6, eaaz1722 (2020).
4. Guo, H. et al. Polymeric ligands comprising sulfur-containing amino acids for targeting tumor-associated amino acid transporters. Biomaterials 293, 121987 (2023).
5. Voon, Y. M. et al. Effect of Spacers on the Affinity of Tyrosine-Modified Polymers to L-Type Amino Acid Transporter 1. Biomacromolecules 26, 2256-2267 (2025).

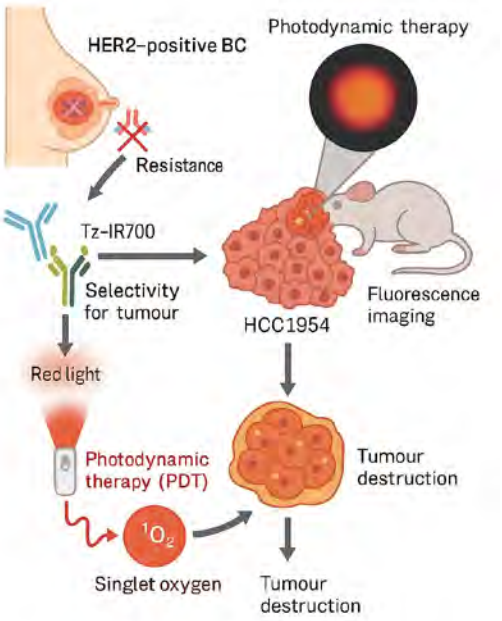
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Photoimmunotherapy with IRDye700DX Bypasses Trastuzumab Resistance in HER2-Positive Breast Cancer

Mireia Jordà-Redondo[a], Ana Piqueras[b], Ana Castillo[b], Pedro Luis Fernández[b], Roger Bresolí-Obach[a], Lidia Blay[b], Joan Francesc Julián Ibáñez[b], *, Santi Nonell[a,c]

[a]*Institut Químic de Sarrià, Universitat Ramon Llull, Barcelona, Spain.*
[b]*Hospital Universitari Germans Trias i Pujol, Badalona, Spain*
E-mail: santi.nonell@iqs.url.edu

Targeted photodynamic therapy (PDT) offers a promising strategy to overcome resistance mechanisms in HER2-positive cancers. In this work, a series of photoimmunoconjugates were engineered by coupling different photosensitisers to trastuzumab and its biosimilar Herzuma®.[1] Comprehensive photophysical and photochemical characterization confirmed that bioconjugation preserves the optical performance of the photosensitisers while conferring selective recognition of HER2-overexpressing tumour cells. Notably, these photoimmunoconjugates exhibited potent photodynamic activity not only in HER2-positive models but also in trastuzumab-resistant cell lines, highlighting their potential to bypass conventional therapeutic resistance. Building on this platform, further functionalization with doxorubicin enabled a dual-action construct capable of light-triggered chemotherapeutic release. This combined modality underscores a versatile approach for enhancing the precision and efficacy of PDT-based cancer treatments and opens new avenues for addressing drug resistance in HER2-driven malignancies.



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REFERENCES

1. Jordà-Redondo, M.; Piqueras, A.; Castillo, A.; Fernández, P.L.; Bresolí-Obach, R.; Blay, L.; Julián Ibáñez, J.F.; Nonell, S. An antibody-photosensitiser bioconjugate overcomes trastuzumab resistance in HER2-positive breast cancer. **Eur. J. Med. Chem.** 2025, 290, 117511.

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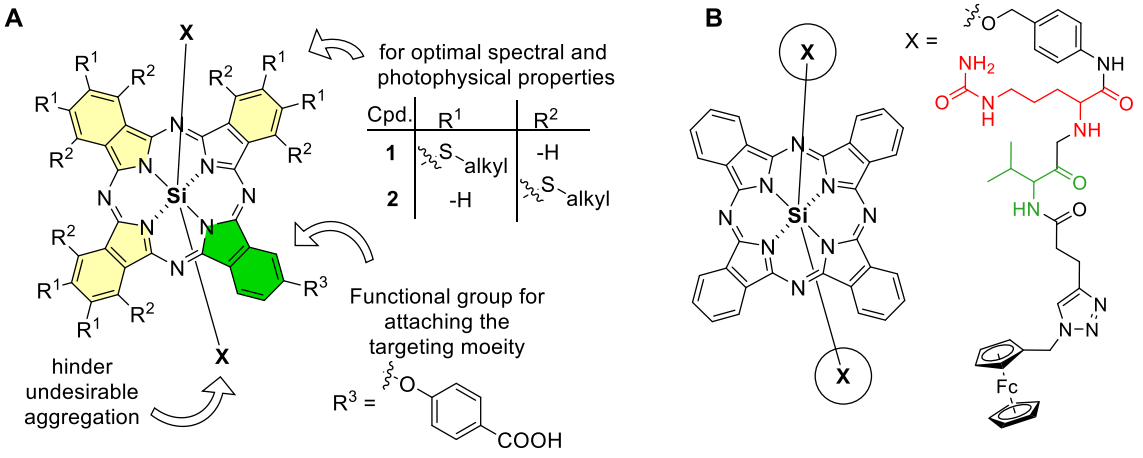
Axial and Peripheral Functionalization of Silicon(IV) Phthalocyanines

Veronika Novakova, Leon David Rodrigues, Mary Angelia Alfred, Petr Zimčík

Faculty of Pharmacy in Hradec Kralove, Charles University, Ak. Heyrovskeho 1203, 500 03 Hradec Kralove, Czech Republic, veronika.novakova@faf.cuni.cz

ORALS

Phthalocyanines (Pcs) have fascinated researchers since their discovery in 1907, which is probably due to their close relationship to naturally occurring porphyrins, available synthesis, and outstanding properties.[1,2] Introduction of Si(IV) into their center brings great advantage in the form of two axial ligands, which effectively prevent undesired aggregation, improve solubility and enable the introduction of a moiety responsible for specific functions.[3]
In my lecture, I will present our latest results in the field of synthesis of low-symetry Si(IV)Pcs, which carry a functional group at their periphery. Thanks to that, they may be simply attached for example to targeting moieties such as aptamers. Axial ligands on the other hand ensure monomeric character and good photophysical properties.
In the second part of my talk, I will focus on modification of axial positions of Si(IV)Pcs with specific ligands that control either the photophysical properties or self-assembly of target macrocycles. As an example, I will show synthesis and study of Si(IV)Pcs carrying a donor for photo-induced electron transfer (PET) attached throug a cathepsine-cleavable linker. It is assumed that cleavage of the linker activates the inactive Si(IV)Pc suppressed by the PET process into a photodynamically active form, primarily in cancer cells due to overexpression of cathepsin in cancer tissues.



The work was supported by the project New Technologies for Translational Research in Pharmaceutical Sciences /NETPHARM, project ID CZ.02.01.01/00/22_008/0004607, co-funded by the European Union.

REFERENCES

1. Lo, P. C.; Rodriguez-Morgade, M. S.; Pandey, R. K.; Ng, D. K. P.; Torres, T.; Dumoulin, F., Chem. Soc. Rev. **2020**, 49, (4), 1041–1056.
2. Claessens, C. G.; Hahn, U.; Torres, T., Chem. Rec. **2008**, 8, (2), 75–97.
3. Lo, P. C.; Huang, J. D.; Cheng, D. Y. Y.; Chan, E. Y. M.; Fong, W. P.; Ko, W. H.; Ng, D. K. P, *Chem. Eur. J.* **2004,** 10, (19), 4831–4838.

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Dissecting the mechanisms of photochemical immunogenic cell death by verteporfin-lipid using unsupervised machine learning

Girgis Obaid[a]

[a] *Fellow, Texas Instruments Catalyst Professor, Assistant Professor of Bioengineering, University of Texas at Dallas, Richardson, Texas, 75080, United States*

Verteporfin, an approved photosensitizer, has been formulated by our team and others' into various lipid-based formulations and molecular conjugates to improve its safety and efficacy [1-3]. Following light activation, verteporfin-based preparations can induce photochemical immunogenic cell death (P-ICD) in cancer cells [4-6]. However, little is known about its mechanisms of action, which hampers the development of more potent verteporfin-based P-ICD agents. To address this critical knowledge gap, we prepared a panel of verteporfin-lipid nanoparticles (V-LNPs) with discrete attributes (subcellular localization, type of photochemical reactions, degree of potency, internalization efficiency etc). Using this panel of V-LNPs that provide a spectrum of well-defined nanoparticle attributes, we investigated their efficiency of P-ICD in multiple pancreatic cancer cell lines. This gave us a high-dimentional dataset describing relationships between V-LNP attributes and their respective efficiencies of inducing P-ICD. Using unsupervised machine learning, we deciphered which of the V-LNP attributes were most strongly associated with P-ICD [7]. Our results, which will be presented at this conference, provide previously unknown insights into which design features of V-LNPs must be prioritized in order to design novel P-ICD agents with the greatest probability of inducing durable anti-tumor immune responses.

REFERENCES

1. Obaid, G., Jin, W., Bano, S., Kessel, D. and Hasan, T. 2019. *Photochemistry and Photobiology*, 95(1), pp.364-377.
2. Obaid, G., Bano, S., Mallidi, S., Broekgaarden, M., Kuriakose, J., Silber, Z., Bulin, A.L., Wang, Y., Mai, Z., Jin, W. and Simeone, D., Lin, C. and Hasan T. 2019. *Nano Letters*, 19(11), pp.7573-7587.
3. Obaid, G., Bano, S., Thomsen, H., Callaghan, S., Swain, J. W. R., Shah, N., Jin, W., Ding, X., Wu, J., Vangel, M., Stoilova-McPhie, S., Zhao, J., Mino-Kenudson, M., Lin, C. and Hasan, T. 2022. *Advanced Science,* 9(24), p.2104594.
4. Bhandari, C., Moffat, A., Shah, N., Khan, A., Quaye, M., Fakhry J., Soma, S., Nguyen, A., Eroy, M., Malkoochi, A., Brekken, R., Hasan, T., Ferruzzi, J. and Obaid, G. 2024. *Advanced Healthcare Materials,* p.2304340.
5. Shah, N., Soma, S.R., Quaye, M.B. Mahmoud, D., Ahmed, S., Malkoochi, A. and Obaid, G. 2024. *ACS Applied Bio Materials*, 7(7), pp.4427-4441.
6. De Silva, P., Bano, S., Pogue, B.W., Wang, K.K., Maytin, E.V. and Hasan, T., 2021. *Nanophotonics*, *10*(12), pp.3199-3214.
7. Shah, N., Quaye, M.B., Soma, S.R., Vadlamudi, M.S., Mahmoud, D., Malkoochi, A., Aileni, T.R., Bhandari, C., Karambelkar, K., Hasan, T., Korbelik, M., Fei, B., Song, X., and Obaid, G. 2025. *Small Science*, *5*(11), p.2500290.

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Porphyrinoid macrocycles as dyes and catalysts for solar energy conversion

Fabrice Odobel,[a]* Diego Defferrari,[a] Stéphane Diring,[a] Paulo Marques-Cordeiro-Junior,[b] Marc Robert[b]

[a]*Nantes Université, CNRS, CEISAM, UMR6230, F-44000 Nantes, France ; E-mail: fabrice.odobel@univ-nantes.fr*
[b]*Sorbonne Université, CNRS, Institut Parisien de Chimie Moléculaire, F-75005 Paris, France*

Porphyrinoids, such as porphyrins and phthalocyanines, rank among the most extensively studied dyes due to their versatile properties for a wide range of applications, including photovoltaics, catalysis, artificial photosynthesis, materials science, and medical therapies. Hybrid macrocycles such as triazabenzoporphyrins or diazabenzoporphyrins are analogues of phthalocyanines, differing by having one or two methylene units instead of a nitrogen atom in meso positions. They exhibit stability and electronic properties comparable to those of phthalocyanines, while offering the distinct advantage of functionalization at the meso carbon positions. While these macrocycles hold promise for the applications stated above, their synthesis poses several challenges, including low yields, labour-intensive purification, and difficulties in scaling up.[1] In this presentation, we first introduce a new methodology that enables the attainment of higher yields and larger quantities of triazabenzoporphyrins than previously existing protocols. In the second part, the catalytic properties of these porphyrinoids towards CO_2 activation, as well as porphyrin systems for photocatalysis, will be presented.

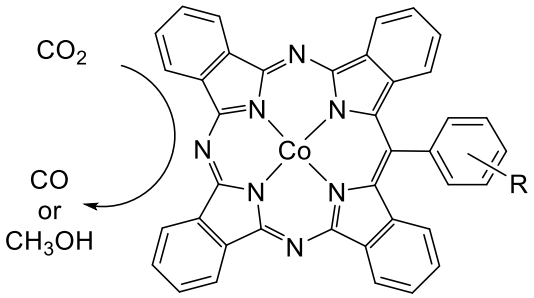


Figure. Structure of a cobalt triazabenzoporphyrin CO_2 reduction catalyst.

REFERENCES

1. (a) N. Alharbi, A. Diaz-Moscoso, G. J. Tizzard, S. J. Coles, M. J. Cook, A. N. Cammidge, Tetrahedron 2014, 70, 7370-7379; (b) A. van As, C. C. Joubert, B. E. Buitendach, E. Erasmus, J. Conradie, A. N. Cammidge, I. Chambrier, M. J. Cook, J. C. Swarts, Inorg. Chem. 2015, 54, 5329-5341; (c) F. Alkorbi, A. Diaz-Moscoso, J. Gretton, I. Chambrier, G. J. Tizzard, S. J. Coles, D. L. Hughes, A. N. Cammidge, Angew. Chem., Int. Ed. 2021, 60, 7632-7636; (d) V. V. Kalashnikov, V. E. Pushkarev, L. G. Tomilova, Mendeleev Commun. 2011, 21, 92-93.

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Monte Carlo and Rate-Equation Modeling of Interstitial Photodynamic Therapy for Brain and Spinal Tumors

Emiyu Ogawa

Keio University, Faculty of Science and Technology, Department of Electronics and Electrical Engineering

ORALS

Interstitial photodynamic therapy (iPDT) using porphyrinoid photosensitizers such as talaporfin sodium is a minimally invasive modality for deep-seated tumors where complete surgical resection is limited by functional risk [1]. Accurate prediction of the effective treatment volume remains challenging due to the coupled dynamics of light transport, photosensitizer activation, and oxygen consumption.

In this study, we developed an integrated *in silico* framework to estimate cytotoxic regions in iPDT for malignant brain and spinal cord tumors. Tissue optical properties were determined experimentally and/or from literature and implemented in three-dimensional Monte Carlo simulations to calculate intratissue fluence distributions [2]. The resulting fluence maps were coupled with a macroscopic singlet oxygen model (MSOM) based on photochemical rate equations to estimate cumulative singlet oxygen production [3]. A threshold singlet oxygen dose was introduced to define the predicted cytotoxic volume. Additionally, oxygen depletion dynamics were incorporated to account for vascular shutdown effects following photochemical reactions. Comparative simulations revealed that differences in tissue optical properties and applicator configurations significantly influence predicted treatment volumes. This computational framework enables quantitative pre-treatment planning of porphyrinoid-based iPDT and provides mechanistic insight into singlet oxygen-mediated cytotoxicity in neural tissues.

REFERENCES

1. Wilson BC, Patterson MS. The physics, biophysics and technology of photodynamic therapy. *Phys Med Biol.* 2008;53(9):R61–R109.
2. Jacques SL. Optical properties of biological tissues: a review. *Phys Med Biol.* 2013;58(11):R37–R61.
3. Wang KKH, Finlay JC, Busch TM, Hahn SM, Zhu TC. Explicit dosimetry for photodynamic therapy: macroscopic singlet oxygen modeling. *J Biophotonics.* 2010;3(5–6):304–318.

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Highly Water-Soluble and Durable Rotaxane-Type Porphyrin Dyes Used as Photosensitizers for Photodynamic Therapy

Yuki Ohishi,[a] **Ichikawa Taiki**,[a] **Masahiko Inouye**[a]

[a] *Graduate School of Medicine and Pharmaceutical Sciences, University of Toyama*

ORALS

Photodynamic therapy (PDT) is an effective cancer treatment that utilizes the generation of reactive oxygen species through light irradiation. Porphyrins are representative photosensitizers, and several of them are already in clinical use for PDT. However, only a few reports of porphyrin derivatives have been reported to simultaneously possess water-solubility, membrane-permeability, and photo-durability, all of which are required for high therapeutic efficacy. In this study, we aimed to apply a rotaxane strategy to porphyrins in PDT (Figure 1).[1] We designed a rotaxane-type photosensitizer **β-Rota**, consisting of a porphyrin axis encapsulated within cyclodextrin (CD). The CD was expected to function as a transparent shell, imparting water solubility and photostability to the porphyrin axis by protecting it from reactive oxygen species.

Based on an efficient synthetic method for rotaxane-type dyes using cucurbit[6]uril (**CB6**),[2] we synthesized **β-Rota** in a high yield by mixing the axial precursor **Axis**, **DM-β-CD**, stopper molecules, and **CB6** in H_2O. **β-Rota** was soluble in aqueous buffers, whereas **Axis** was insoluble. The sensitizing ability of **β-Rota** was evaluated by using a $^1O_2$ scavenger. **β-Rota** exhibited high sensitizing ability comparable to tetraphenylporphyrin tetrasulfonic acid (TPPS), which is known for its high $^1O_2$ generation performance, proving that **β-Rota** sufficiently works as a photosensitizer even though the porphyrin core is encapsulated by the CD shells. A stability test under continuous photoirradiation demonstrated significantly higher photostability of **β-Rota** than a reference rotaxane lacking CD shells. In in vitro assays, **β-Rota** showed higher cell membrane-permeability and photocytotoxicity than talaporfin sodium, a clinically used photosensitizer. These results indicate that the rotaxane-type porphyrin dyes have strong potential as ideal PDT drugs.

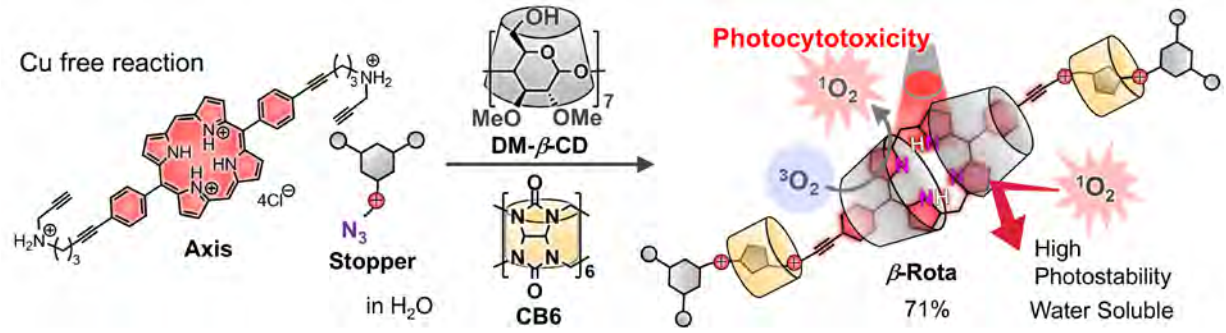


Figure 1. Synthesis and properties of rotaxane-type photosensitizer **β-Rota**.

REFERENCES

1. Y. Ohishi et al. *ACS Appl. Bio Mater.* **2024**, *7*, 6656–6664.
2. Y. Ohishi et al. *Adv. Opt. Mater*. **2024**, *12*, 2301457; *Chem. Sci.* **2025**, *16*, 20414–20421.

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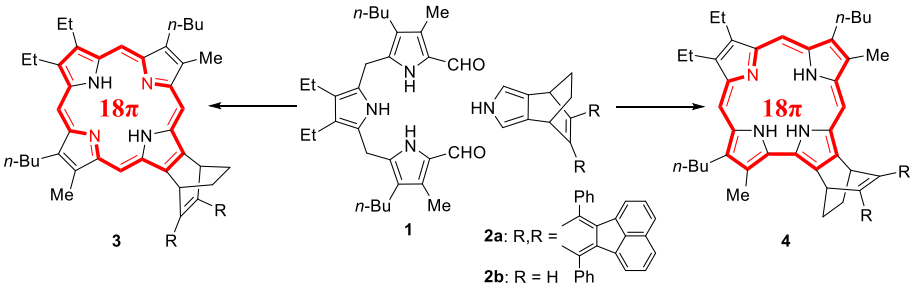


Serendipitous formation of *meso*-free corroles via [3+1] approach and its oxidation to *meso*-oxoisocorroles

Tetsuo Okujima

Graduate School of Science and Engineering, Ehime University, 790-8577 Japan

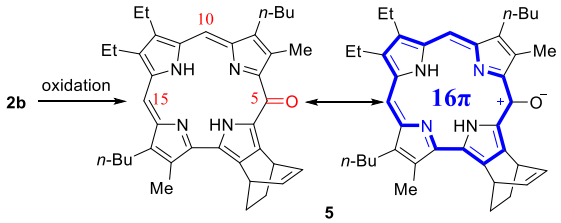
Meso-free corroles are commonly synthesized via pyrrole tetramerization or the ring-closure of tetrapyrrolic intermediate such as biladiene. Other methods include condensation of dipyrranes with 2,2'-bipyrroles or contraction of thiaphlorins.



Recently, we reported that the [3+1] porphyrin synthesis unexpectedly afforded *meso*-free corroles during the preparative investigation of π-extended porphyrinoids based on the retro Diels–Alder strategy from thermally convertible precursors.[1]

Acid-mediated [3+1] porphyrin synthesis using diformyltripyrrane **1** and bicyclo[2.2.2]octadiene(BCOD)-fused pyrroles **2a** in $CHCl_3$ afforded trace amounts of porphyrin **3a** and corrole **4a** in 12% yield. Examination of the reaction conditions revealed that the presence or absence of ethanol in the reaction solvent affected the formation of corrole and porphyrin, respectively. The [3+2] sapphyrin synthesis resulted in the formation of 5-pyrrolylcorrole and isosmaragdyrin, along with the originally targeted sapphyrin.

Tanaka *et al*. experimentally demonstrated the 16π antiaromatic character of 5,15-diaryl-10-oxoisocorrole.[3] Nardis *et al*. reported the synthesis of 5- and 10-oxoisocorroles via the oxidation of symmetrical *meso*-free *β*-octaalkylcorroles.[4] Asymmetric corrole **2b** was oxidized with MnO_2 to afford 5-, 10-, and 15-oxoisocorroles. The ^1H NMR spectrum of **5** exhibited inner NH signals and *meso*-CH signals at 22.50 and 22.01 ppm, and 5.38 and 4.95 ppm, respectively, due to a paratropic ring current effect. Absorption spectra and theoretical calculations supported the antiaromatic character based on a 16π conjugation pathway.



REFERENCES

1. Uno H, Konishi S, Nakamura J, Mori S, Takase M and Okujima T. *J. Porphyrin Phthalocyanines* 2023; **27**: 274-284.
2. Ueta K, Kim J, Ooi S, oh J, Shin J, Nakai A, Lim M, Tanaka T, Kim D and Osuka A. J. Am. Chem. Soc. 2021: 143: 7958-7967.
3. Di Zasso L, Nardis S, Caroleo F, Pizzoli F, Fronczek FR, Smith KM, Berna BB and Paolesse R. Chem. Commun. 2024 ; 60 : 102-105.
4. Okujima T, Takahashi K, Konishi S, Mori S, Nakamura J, Fukunaga S, Uno H and Takase M. *J. Porphyrin Phthalocyanines* 2025; **29**: 1107-1111.

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Porphyrin–Gold Nanoaggregates as Multifunctional Platforms for Photothermal Cancer Therapy

G. Oliviero[a], N. Borbone[b], S. D'Errico[b], L. De Stefano[c], A. D'urso[d], M.G. Nolli[b], M. Terracciano[b], G. Piccialli[b]

[a]*Department of Molecular Medicine and Medical Biotechnology, University of Naples Federico II, 80131 Naples, Italy*
[b]*Department of Pharmacy, University of Naples Federico II, 80131 Naples, Italy*
[c] *Institute of Applied Sciences and Intelligent Systems "E. Caianiello" (ISASI), National Research Council (CNR), 80131 Naples, Italy*
[d]*Department of Chemical Sciences, University of Catania, 95125 Catania, Italy*

We present a new class of hybrid gold–porphyrin nanoaggregates engineered through a one-pot chemical reduction method to maximize photothermal performance for cancer therapy. The nanostructures exploit the synergistic interplay between the localized surface plasmon resonance of gold and the π-conjugated porphyrin chromophore,[1] enabling enhanced absorption in the near-infrared region.
The assembly is driven by electrostatic interactions between $AuCl_4^-$ and cationic amino-functionalized porphyrins (C3, C5 linkers), followed by $NaBH_4$ reduction in the presence of PEG to ensure colloidal stability and biocompatibility. The resulting nanoaggregates (>100 nm) exhibit excellent stability in physiological media and good hemocompatibility.
Comprehensive structural and spectroscopic analyses (^{1}H NMR, DLS, TEM, EDS, UV–Vis, fluorescence) confirm the successful formation of the hybrid interface and the strengthening of plasmon–chromophore coupling. This effect significantly improves photothermal conversion efficiency under NIR irradiation. Moreover, the intrinsic protonation of the modified porphyrin at physiological pH provides a robust anchoring site for targeting aptamers,[2,3] expanding the potential for selective cancer cell recognition.
Overall, these results highlight gold–porphyrin nanoaggregates as versatile and promising platforms for targeted photothermal cancer therapy.

REFERENCES

1. H. Sheng, J. Wang, J. Huang, Z. Li, G. Ren, L. Zhang, L. Yu, M. Zhao, X. Li, G. Li, N. Wang, C. Shen, G. Lu, *Nat. Commun.*, 2023, *14*, 1528.
2. A. D'Urso, R. Randazzo, V. Rizzo, C. Gangemi, V. Romanucci, A. Zarrelli, G. Tomaselli, D. Milardi, N. Borbone, R.Purrello, G. Piccialli, G. Di Fabio, G. Oliviero, *Phys. Chem. Chem. Phys*, 2017, *19*, 17404-17410.
3. A.P. Falanga, A. D'Urso, G. Travagliante, C. Gangemi, M. Marzano, S. D'Errico, M. Terracciano, F. Greco, L. De Stefano, P. Dardano, I. Rea, G. Piccialli, G. Oliviero, N. Borbone.

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Al(III)-based Dinuclear Triple-Stranded Helicates for Diverse Photofunctions

Toshikazu Ono[a,b]

[a]*Graduate School of Engineering, Kyushu University*
[b]*Center for Molecular Systems (CMS), Kyushu University*

ORALS

Pyrrole-based π-conjugated frameworks continue to play a central role in the development of functional dyes due to their structural modularity, tunable electronic properties, and strong coordination ability. Building on this concept, our group have developed aluminum(III) complexes supported by pyrrole-derived ligands as a new platform for sustainable photofunctional materials. Although aluminum is abundant, inexpensive, and low-toxicity, the photophysics of Al-based π-systems remain underdeveloped, making them attractive targets for establishing structure–property relationships. Here, we present a series of Al(III)-based dinuclear triple-stranded helicates constructed from three ligands and two Al(III) ions.[1,2] Systematic modification of the ligands allows for continuous tuning of the emission color from blue to the near-infrared (NIR) region under UV excitation (Figure 1). X-ray crystallographic analysis and DFT calculations reveal that the twist angle of the ligands is the key structural parameter governing the emission energy. In the solid state, mechanical grinding perturbs the ordered π-stacking motifs of the helicates, inducing a reversible crystalline-to-amorphous transition and resulting in pronounced mechanochromic shifts in both absorption and emission spectra.[3] Furthermore, the combinations of electron-donating and electron-withdrawing ligands generate inter-ligand charge-transfer (ILCT) states, which, assisted by internal heavy-atom effects, promote efficient triplet formation and singlet-oxygen generation.[4] These properties also enable the application of the helicates as catalysts for singlet-oxygen-mediated reactions. We will also discuss transient absorption studies that provide deeper insight into the excited-state dynamics of these pyrrole-based helicates.

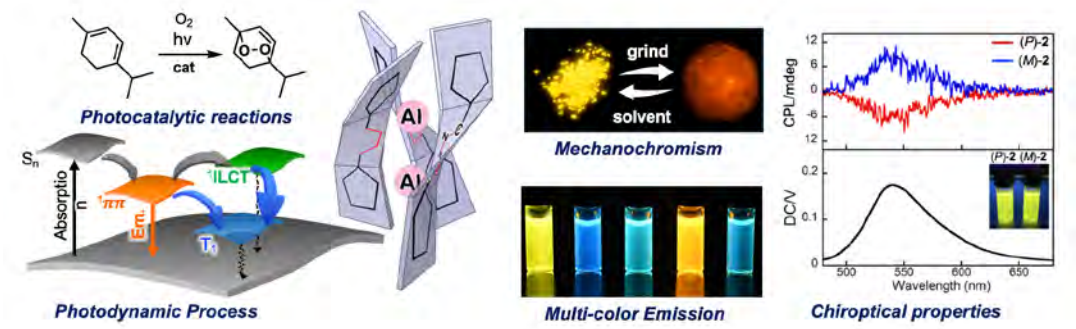


Figure 1. Diverse functions exhibited by the Al(III)-based triple-stranded helicates used in this study.

REFERENCES

1. T. Ono and K Ishihama et al., *Angew. Chem. Int. Ed.* **2021**, *60*, 2614.
2. K. Ueno and T. Ono et al., *Inorg. Chem.* **2024**, *63*, 6296.
3. T. Umeki and T. Ono et al., *submitted.*
4. Y. Konishi and T. Ono et al., I*norg. Chem.* **2024**, *63*, 11716.

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Engineered Hemoprotein Containing Ni Tetradehydrocorrin as an Artificial Cofactor

Koji Oohora[a]

[a]*Department of Applied Chemistry, Graduate School of Engineering, The University of Osaka,2-1 Yamadaoka, Suita, 565-0871 Japan*

In biological systems, a wide variety of metalloproteins have been identified. In particular, hemoproteins exhibit diverse and unique functions, including electron transfer, gas binding, and catalysis. In hemoproteins, the physicochemical properties and reactivity of the common cofactor heme are strongly governed by the surrounding protein matrix, which plays a critical role in regulating heme function [1]. Motivated by this unique feature, our group has explored and expanded hemoprotein systems by incorporating artificial heme derivatives. For example, manganese and iron porphyrinoids have been inserted into the apo-form of myoglobin, a simple oxygen-binding hemoprotein, to create artificial metalloenzymes capable of C–H bond hydroxylation [2] and olefin cyclopropanation [3], respectively. Similarly, myoglobins reconstituted with cobalt tetradehydrocorrins have been developed as functional models of methionine synthase [4].

Understanding enzymatic reaction mechanisms provides valuable insights into the molecular design of artificial biocatalysts for environmentally friendly reactions. In this context, we have recently focused on methyl-coenzyme M reductase (MCR), a key enzyme responsible for biological methane formation. MCR contains F430, a nickel tetrapyrrole complex, as its cofactor [5]. Although a Ni(I) species has been proposed as the catalytically active intermediate, the detailed reaction mechanism remains unclear due to the structural complexity of the enzyme. Moreover, functional models that explicitly incorporate a protein matrix have not yet been reported. To address this challenge, the present study describes the preparation and evaluation of protein-based functional models of MCR through conjugation of nickel complexes with protein matrices.

Nickel tetradehydrocorrin (Ni(TDHC)) and nickel didehydrocorrin (Ni(DDHC)) were employed as model complexes of F430, while apo-hemoproteins derived from myoglobin (Mb) and cytochrome b_{562} (Cyt b_{562}) were used as protein matrices. Conjugation of Ni(TDHC) with the apo-form of Mb afforded a reconstituted Mb, which exhibited catalytic methane formation from methyl iodide. In contrast, Ni(TDHC) alone, in the absence of a protein matrix, did not promote the reaction, clearly demonstrating the essential role of the protein scaffold.

In parallel, reconstituted Cyt b_{562} was prepared by conjugation of Ni(DDHC) with the apo-form of Cyt b_{562}. Under photoirradiation in the presence of a photosensitizer, methane formation via cleavage of the C–S bond of a methionine residue in reconstituted Cyt b_{562} was observed.

REFERENCES

1. K. Oohora, T. Hayashi, *Dalton Trans.* **2021**, *50*, 1940-1949.
2. K. Oohora, H. Meichin, Y. Kihira, H. Sugimoto, Y. Shiro, T. Hayashi, *J. Am. Chem. Soc.* **2017**, *139*, 18460-18463.
3. Y. Kagawa, K. Oohora, T. Himiyama, A. Suzuki, T. Hayashi, *Angew. Chem. Int. Ed.* **2024**, *63*, e202412565.
4. Y. Morita, K. Oohora, A. Sawada, T. Kamachi, K. Yoshizawa, T. Hayashi, *Inorg. Chem.* **2017**, *56*, 1950-1955.
5. K. Oohora, Y. Miyazaki, T. Hayashi, *Angew. Chem. Int. Ed.* **2019**, *58*, 13813-13817.

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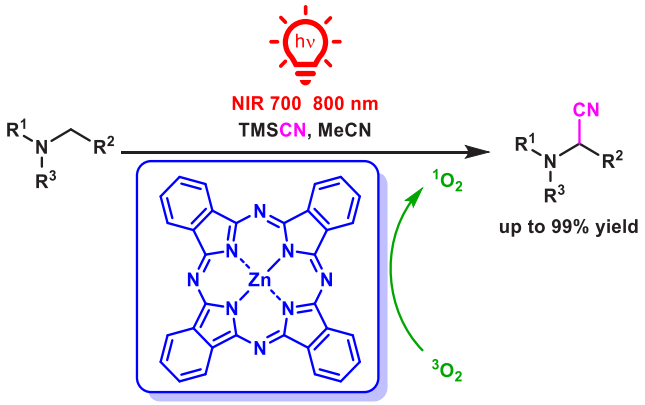
Photochemical α-Aminonitrile Synthesis Using Zn-Phthalocyanines as Near-Infrared Photocatalysts

Till Opatz[a], Caroline Grundke[a], Rodrigo C. Silva[b], Winald R. Kitzmann[a], Katja Heinze[a], Kleber Thiago de Oliveira[b]

[a]*Department of Chemistry, Johannes Gutenberg University Mainz, Duesbergweg 10-14, 55128 Mainz, Germany.*
[b]*Departamento de Química, Universidade Federal de São Carlos, São Carlos, SP 13565905, Brazil.*

ORALS

While photochemical transformations with sunlight almost exclusively utilize the UV-Vis part of the solar spectrum, the majority of the photons emitted by the sun have frequencies in the near-infrared region. Phthalocyanines show structural similarity to the naturally occurring light harvesting porphyrins, chlorins and mainly bacteriochlorins, and are also known for being efficient and affordable near-infrared light absorbers as well as triplet sensitizers for the production of singlet oxygen. Although having been neglected for a long time in preparative organic photochemistry, presumably due to their low solubility and high tendency towards aggregation, their unique photophysical properties and chemical robustness make phthalocyanines attractive photocatalysts for the application in near-infrared light-driven synthesis strategies.
We developed a cheap, simple and efficient photocatalytic protocol, which is easily scalable under continuous flow conditions. Various phthalocyanines were studied as near-infrared photosensitizers in oxidative cyanations of tertiary amines to generate α-aminonitriles, a synthetically versatile compound class.[1]



REFERENCES

1. C. Grundke, R. Silva, W. Kitzmann, K. Heinze, K. de Oliveira, T. Opatz, *J. Org. Chem.,* **2022**, *87*, 5630–5642.

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Influence of geometrical factors on ECD spectra of porphyrin-based supramolecules

I. Osadchuk, V. Borovkov

Tallinn University of Technology, Department of Chemistry and Biotechnology

ORALS

Electronic circular dichroism (ECD) spectroscopy is a widely used chiroptical method for determining the absolute configuration of chiral molecules [1-2]. A major limitation of ECD spectroscopy is the requirement for a chromophore located close to the chiral center; however, many organic molecules do not satisfy this condition. To overcome this limitation, chirality is often determined using the ECD spectra of complexes formed between the molecule under study and a porphyrinoid.

ECD spectra are straightforward to measure; however, for compounds containing multiple chromophores and complex stereochemistry, the interpretation of ECD spectra becomes challenging. Therefore, experimentally measured ECD spectra are now frequently combined with computational studies. From a computational chemistry perspective, an important consideration is that ECD spectra are conformation-dependent. Therefore, spectral simulations are always preceded by a conformational search—a time-consuming, resource-intensive procedure. Importantly, with increasing molecular size, both computational costs and the risk of overlooking important molecular conformations increace.

Our goal was to identify molecular fragments that contribute minimally to the ECD spectrum and to simplify the molecular structure by replacing them with smaller ones (ideally hydrogen atoms). In this context, the effect of the relative orientation of the molecule with respect to the porphyrin was investigated (Figure 1), as well as the manner in which conformational changes of the porphyrin and organic molecules are reflected in the spectrum. Furthermore, the influence of secondary chromophores and porphyrin substituents with electron-donating and electron-withdrawing properties was systematically studied studied. Calculations were performed using semi-empirical, DFT, and TD-DFT approaches.

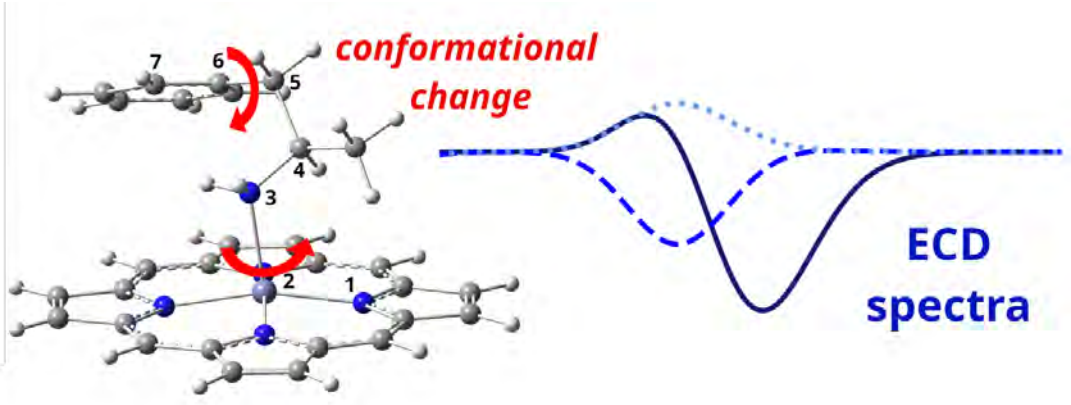


Figure 1. How conformational change can influence ECD spectra of porphyrin-based supramolecule.

REFERENCES

1. Polavarapu, P. L. *Chirality* 24, (**2012**), 909–920.
2. A. Mándi, T. Kurtán, *Nat. Prod. Rep*., 36, (**2019**), 889–918.

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Trial of photodynamic therapy for canine bladder transitional cell carcinomas

Tomohiro Osaki[a], Shuntaro Tao[a], Isao Sakata[b], Kiwamu Takahashi[c], Takashi Iwasaki[a], Tetsuya Kadonosono[d], Takahiro Nomoto[e]

[a] *Faculty of Agriculture, Tottori University, Tottori, Japan*
[b] *JS-Stage, Okayama, Japan*
[c] *SBI Pharmaceuticals Co., Ltd., Tokyo, Japan*
[d] *School of Life Science & Technology, Institute of Science Tokyo, Kanagawa, Japan*
[e] *Graduate School of Arts and Sciences, The University of Tokyo, Japan*

Background and Objective
Most canine bladder tumors are transitional epithelial carcinomas (TCCs), often treated by surgical resection. However, if the lesion occurs in the bladder triangle, the urinary tract must be secured, necessitating cystectomy and urinary tract alteration[1]. Recently, photodynamic therapy (PDT) has attracted attention as a novel cancer treatment option. This treatment method destroys tumors by applying laser irradiation to the affected tumor area after administering a tumor-accumulating photosensitizing agent. In the present study, PDT was performed to preserve bladder function in 15 canines diagnosed with TCC, and relatively good results were obtained. We also developed pheophorbide A (Pa)-conjugated HER2-targeted NBs (Pa-NB conjugates) and evaluated the cytotoxicity induced by PDT using Pa-NB conjugates for TCC cells *in vitro*.
Materials and Methods
Clinical trial: Fifteen dogs with TCCs were treated with PDT. The photosensitizers used were 5-aminolevulinic acid hydrochloride (5-ALA), a precursor of the photosensitizer protoporphyrin IX, and PAD-S31, a newly developed hydrophilic photosensitizer. *In vitro* study: TCC cells were incubated with a dilution series of Pa, Pa-bovine serum albumin (BSA) conjugates, and Pa-NBs conjugates for 1 h at 37°C. After incubation, the cells were irradiated with 670 nm LED light.
Results and Discussion
Clinical trial: The objective response rate to PDT was 82%. In many cases, mild gastrointestinal and cystitis-like symptoms were observed on the day of treatment or for several days after treatment. In some cases, treatment had to be discontinued because of hydronephrosis caused by TCC infiltration into the ureter. The median survival time upon reporting, including the seven animals undergoing treatment, was 286 days (median: 108−1,401 days). Repeated PDT enables control of TCCs, suggesting that PDT may be a new treatment method for bladder TCCs. *In vitro* study: Pa-NB conjugates induced cell death in a concentration-dependent manner in TCC cells expressing high levels of HER2. Upon laser irradiation, the Pa-NB conjugates selectively induced significant cytotoxicity in HER2-positive cells.
Conclusions
We plan to evaluate the usefulness of PDT for bladder TCC by increasing the number of cases and continuing to develop PDT with higher therapeutic effectiveness and fewer side effects. Therefore, Pa-NB conjugates may be a new, attractive therapeutic modality for the treatment of HER2-positive cancers.

REFERENCES

1. Fulkerson CM, Knapp DW. Management of transitional cell carcinoma of the urinary bladder in dogs: a review. Vet J. 2015 Aug;205(2):217-25.

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Stable Antiaromatic Expanded Porphyrins

Yutao Rao[a], Ling Xu[a], Mingbo Zhou[a], Atsuhiro Osuka[a], and Jianxin Song[a]

[a]*College of Chemistry and Chemical Engineering, Hunan Normal University, Changsha 410081, China*

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Porphyrinoids including porphyrins and expanded porphyrins have been usually synthesized by acid-catalyzed condensation reactions of pyrroles and oligopyrroles with aldehydes and their equivaents so far. In recent years, we have explored our original non-condensation synthetic methods that allow for the synthesos of novel expanded porphyrins. Our methods rely on Pd(II)-catalyzed Suzuki-Miyaura cross coupling, S_NAr reaction of α,α'-dibromo-oligopyrrin with *meso*-aryl dipyrromethane or tripyrromethane, and Friedel-Crafts type electrophilic aromatic substitution reaction of *meso*-aryl dipyrromethane or tripyrromethane with α,α'-dibromo-oligopyrrin. In this presentation, we will report several representative examples. Curiously we often obtained antiaromatic expanded porphyrins as the most stable products. 5,10,23-Trimesityl-substituted [24]hexaphyrin(1.1.0.0..1.0) was synthesized by S_NAr reaction of α,α'-dibromo-5.10-dimesiyltrypyrrane with a tripyrrolic compound. This hexaphyrin shows signals due to the outer pyrrolic β-protons in the range of 4.76 ~ 3.78 ppm. Its bis-Pd(II) complex shows a stronger paratropic ring current by displaying signals due to the outer β-protons in the range of 2.40 ~ 0.70 ppm.[1] On the other hand, 5,10,23-trimesityl-substituted [28]heptaphyrin(1.1.0.0.1.0.0) was synthesized by *p*-toluenesulfonic acid catayzed reaction between tetrapyrrolic BF_2 complex and α,α'-dibromo-5.10-dimesiyltrypyrrane. A very strong paratropic ring current was observed for its bis-Pd(II) complex, which shows signals due to the outer β-pyrrolic protons in the range of -1.06 ~ -1.90 ppm as a rare case.[2] A mixture of 5,18-dimesityl[20]orangrin and its BF_2 complex was obtained by S_NAr reaction of 5-mesityl-α,α'-dibromo BODIPY with a tripyrrolic compound.[3] The free base orangarin shows signals due to the outer β-protons in the range of 4.29 ~ 3.82 ppm and its BF_2 complex (these [20]orangarins are called as 3*NH*-orangarin since they have three inner pyrrolic NH protons) shows those in the range of 4.82 ~ 3.12 ppm. The BF_2 complex was transformed into a cyclooctatetrane(COT)-centered orangarin dimer via selective β-bromination, Ni(0)-catalyzed reductive coupling, and oxidative fusion reaction with DDQ and $Sc(OTf)_3$. The COT-centered [20]orangarin dimer was further dimerized by oxidation with MnO_2 to give COT-centered [20]orangarin tetramer. The COT-centered [20]orangarin dimer and tetramer were mildly oxidized with MnO_2 to produce the corresponding dimer and tetramer consisting of 2*NH*-orangarins, which display characteristic strong absorption bands around 1000 ~ 1100 nm.

REFERENCES

[1] Y. Liu, L. Xu, Y. Rao, J. Kim, M. Zhou, J. Oh, D. Kim, J. Song, A. Osuka, *Org. Lett.* **2023**, *25*, 8121.
[2] Y. Liu, L. Xu, X. Jin, B. Yin, Y. Rao, M. Zhou, J. Song, A. Osuka, *Chem. Sci.* **2024**, *15*, 11402.
[3] Y. Rao, J. Lee, J. Chen, L. Xu, M. Zhou, B. Yin, J. Kim, A. Osuka, J. Song, *Angew. Chem. Int. Ed.* **2024**, *63*, e202409655.

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Face-to-Face Porphyrin Dimers via Coordination and Dynamic Covalent Bonding

Joe Otsuki[a]

[a]*College of Science and Technology, Nihon University, 1-8-14 Kanda Surugadai, Chiyoda, Tokyo 101-8308 Japan, +81-3-3259-0817, otsuki.joe@nihon-u.ac.jp*

Cofacial porphyrin dimers represent a promising class of supramolecular architectures for molecular recognition, catalysis, and sensing applications. We developed a series of zinc porphyrins bearing chelating ligands at the *meso*-phenyl positions that undergo cooperative, metal-ion-driven dimerization to yield face-to-face assemblies. The parent compound, ZnPor(bpy)$_4$, forms a stable dimer through coordination of four Zn^{2+} ions, exhibiting a distinct S-shaped titration curve that reflects cooperative Zn^{2+} binding [1] (Figure 1). UV–vis, NMR, ESI-MS, and single-crystal X-ray analyses confirmed the tetrahedral Zn(bpy)$_2$ coordination geometry linking the two porphyrin units at an interplanar separation of ~5 Å. The resulting dimer is remarkably stable, persisting even under dilute or excess-metal conditions.

To enhance the structural rigidity and metal-binding strength of this system, the bipyridine ligand was replaced with more rigid 1,10-phenanthroline groups, affording ZnPor(phen)$_4$, which forms even more robust metal-ion-bridged dimers [2]. The phenanthroline framework enhances cooperative assembly and structural rigidity, as verified by MCR-ALS analysis, DOSY NMR, and ESI-MS analyses, revealing tetrahedral M(phen)$_2$ linkages with interporphyrin distances of 5.7–6.2 Å.

To introduce accessible cavities, acetylene- and diacetylene-extended derivatives, ZnPor(C_2bpy)$_4$ and ZnPor(C_4bpy)$_4$, were also synthesized. These form Zn^{2+}-bridged cofacial dimers with increased interplanar distances estimated from ^{1}H NMR data to be ~9 Å and ~13 Å, respectively. The larger ZnPor(C_4bpy)$_4$ dimer acts as a host molecule, selectively encapsulating 4,4'-bipyridine with a high association constant on the order of 10^5 M^{-1}, demonstrating size-selective host-guest recognition.

Beyond coordination-driven assembly, dynamic covalent chemistry was also explored as a complementary route to thermodynamically stable architectures. An imine-forming reaction between a tetraaminoporphyrin and 2,6-diformylpyridine afforded a cage compound capable of encapsulating C_{60} within its cavity.

These studies establish a versatile molecular design concept for constructing cavity-defined porphyrin dimers through either coordination or covalent dynamic bonding. Such supramolecular systems provide versatile platforms for switchable host–guest systems and multi-metal catalytic assemblies.

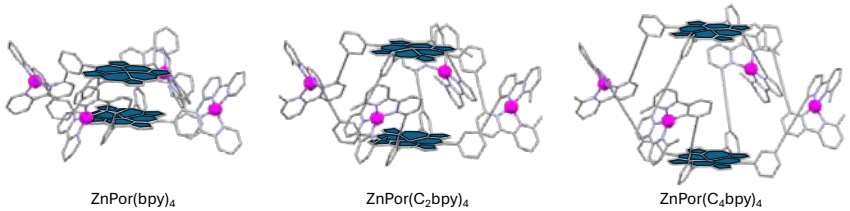


Figure 1. Coordination-driven porphyrin dimers with different interporphyrin distances.

REFERENCES

1. J. Otsuki, K. Sato, K. Sugawa, *Eur. J. Inorg. Chem.* **2024**, *27*, e202400188.
2. J. Otsuki, K. Sato, Y. Nakaie, Y. Hosoya, K. Sugawa, *Chem. Lett.* DOI: 10.1093/chemle/upaf182.

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From H_3^+ to Porphyrinoids: An Excursion into the Wide Land of Excited State Aromaticity and Antiaromaticity

Henrik Ottosson [a]

[a] *Department of Chemistry – Ångström Laboratory, Uppsala University, Box 523, 751 20 Uppsala, Sweden.*

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During the last decades, it has gradually become recognized that aromaticity and antiaromaticity impact on a number of different properties and processes in the lowest electronically excited states.[1-4] Yet, it was concluded already by Colin Baird in his pioneering 1972 paper that "*The antiaromaticity associated with the triplet state of benzenoid hydrocarbons is predicted to yield drastic changes in the intermolecular reactivity compared to the ground state*".[5] We now know that the excited state aromaticity and antiaromaticity concepts (ESA & ESAA) can be applied widely; from H_3^+,[6] the smallest and most abundant aromatic species in the Universe, to expanded porphyrins and other macrocycles.[7-9] Simultaneously, we also gradually unravel the limitations, complications and pitfalls of the concepts, realizing that some molecules are Hückel-aromatic in their lowest excited states instead of Baird-aromatic,[10] and that nπ* states of heteroaromatics exhibit tug-of-wars between antiaromatic $2n$ π_α spin-components and aromatic $2n+1$ π_β spin-components which either result in a residual aromatic or antiaromatic character.[11,12] In this talk, I will exemplify the wide utility of the ESA & ESAA concepts in studies that span from the small triangular H_3^+ cation to large porphyrinoids. What general conclusions can be drawn on aromaticity and antiaromaticity effects in electronically excited states? How widely applicable are the concepts, and when do we need to be cautious?

REFERENCES

1. H. Ottosson, *Nat. Chem.* **2012**, *4*, 929-931.
2. M. Rosenberg, C. Dahlstrand, K. Kilså, H. Ottosson, *Chem. Rev.* **2014**, *114*, 5379-5425.
3. L. J. Karas, J. I. Wu, *Nat. Chem.* **2022**, *14*, 723-725.
4. J. Yan, T. Slanina, J. Bergman, H. Ottosson, *Chem. Eur. J.* **2023**, *29*, e202203748.
5. N. C. Baird, *J. Am. Chem. Soc.*, **1972**, *94*, 4941-4948.
6. J. Toldo, J. Staab, E. Matito, C. Foroutan-Nejad, H. Ottosson, *Chem. Sci.*, **2026**, DOI: 10.1039/d5sc09067a
7. Y.M. Sung, M.-C. Yoon, J. M. Lim, H. Rath, K. Naoda, A. Osuka, D. Kim, *Nat. Chem.*, **2015**, *7*, 418-422.
8. J. Kim, J. Oh, A. Osuka, D. Kim, *Chem. Soc. Rev.*, **2022**, *51*, 268-292.
9. R. Ayub, O. El Bakouri, J. R. Smith, K. Jorner, H. Ottosson, *J. Phys. Chem. A*, **2021**, *125*, 570-584.
10. W. Zang, O. El Bakouri, D. W. Szczepanik, H. Bronstein, H. Ottosson, *Chem. Sci.* **2021**, *12*, 6159-6171.
11. N. Proos-Vedin, S. Escayola, S. Radenkovic, M. Solà, H. Ottosson, *J. Phys. Chem. A*, **2024**, 128, 4493-4506.
12. N. Proos-Vedin, J. Toldo, S. Escayola, S. Radenkovic, M. Solà, H. Ottosson, *J. Org. Chem.*, **2025**, 90, 9743-9756.

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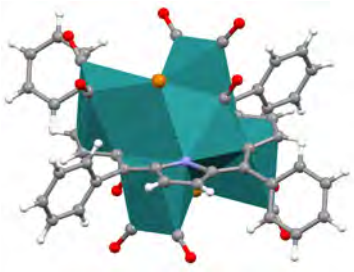
Porphyrin—ruthenium cluster hybrids

Ewa Pacholska-Dudziak[a], **Paulina Krzyszowska**[a], **Emilia Ganczar**[a]

[a]*University of Wroclaw, Faculty of Chemistry, ul. Joliot-Curie 14, Wrocław, Poland*

The replacement of skeleton atoms of a porphyrin with other atoms results in the formation of heteroporphyrins. A distinctive subclass of heteroporphyrins is that of 21-metallaporphyrins, which feature a metal atom in the position of one or two inner nitrogens of the porphyrin macrocycle. To date, a series of 21-metalla-23-tellurporphyrins have been discovered, where the metal is Pd(II), Pt(II), Pt(IV) and Rh(III), and 21,23-dimetallaporphyrins, in which two metal ions in the porphyrin core are located in close proximity. Depending on the electron configuration of the metal ion, metal-metal interaction may or may not be observed. [1] The synthesis of the aforementioned compounds utilises 21,23-ditellurporphyrins as substrates. Metallaporphyrins exhibit macrocyclic aromaticity characteristic of porphyrins, as evidenced by spectroscopic analysis. Interestingly, unusual metallaantiaromaticity was observed for a differently constructed metallaporphyrinoid, 10-platinacorrole complexes, obtained in H. Shinokubo group.[2]

The use of ruthenium, an element capable of forming π-bonds with the porphyrin skeleton, within the context of metallaporphyrins, led us to obtain a whole series of compounds that can be categorised as porphyrin-metal cluster hybrids. These compounds consist of a 21,23-diruthenaporphyrin macrocycle to which additional ruthenium atoms are attached and stabilised by extra bridges and ligands. These systems are characterised by their high rigidity and specific spectroscopic properties.



Ruthenium was also used in a synthesis based on tetratellurooctapyrin to obtain an expanded metallaporphyrin. However, in this case, the crucial reaction in the synthesis of ruthenaporphyrins — converting tellurophene to ruthenacyclopentadiene — terminated at an earlier stage. This resulted in the formation of a stable model of an intermediate product in metallaporphyrin synthesis, containing both ruthenium and tellurium within a 6-membered ring. [3]

REFERENCES

1. E. Pacholska-Dudziak, M. Szczepaniak, A. Książek, L. Latos-Grażyński, *Angew. Chem. Int. Ed.* **201**, *52*, 8898; E. Pacholska-Dudziak, G. Vetter, A. Góratowska, A. Białońska, L. Latos-Grażyński, *Chem. Eur. J.*, **2020**, *26,* 1601; G. Vetter, A. Białońska, P. Krzyszowska, S. Koniarz, E. Pacholska-Dudziak, *Chem. Eur. J,* **2022**, *28,* e202201513; G. Vetter, A. Białońska, A. Jezierska, J. J. Panek, E. Pacholska-Dudziak, *Chem. Commun.*, **2023**, *59*, 6841.
2. Miwa, K.; Yokota, T.; Wang, Q.; Sakurai, T.; Fliegl, H.; Sundholm, D.; Shinokubo, H. *J. Am. Chem. Soc.* **2024**, *146*, 1396; S. Kato, K. Miwa, H. Takano, H. Shinokubo, *Inorg. Chem.* **2025**, *64*, 10916.
3. Krzyszowska, P.; Ganczar, E.; Chmielewski, P. J.; Pacholska-Dudziak, E. *Inorg. Chem.* **2024**, *63*, 21788.

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Enzyme-like Polymers: A synthetic approach to mimicking multimeric hemoproteins

Hannah Palomino[a], Aaron Shoemaker[a], Sabrina El-Gamal[a], Cybele Lemuh Njimoh[b], Nicolai Lehnert[b], Bryan Hunter[a], Karl Scheidt[a], Nathan Gianneschi[a]

[a]*Department of Chemistry, Northwestern University, Evanston, IL 60208, USA.*
[b]*Department of Chemistry, University of Michigan, Ann Arbor, MI 48109, USA.*

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Despite advances in mimicking and tailoring hierarchical protein structure through protein engineering, de novo design, and simplified peptide-based mimetics, reducing the complexity of the protein matrix without compromising stability and function remains a fundamental challenge.[1–3] Guided by comparative active-site analysis across hemoproteins, we designed enzyme-like polymers (ELPs) based on the conserved helix–heme–helix motif using solid-phase peptide synthesis and ring-opening metathesis polymerization.[4,5] Using a 40-amino acid active-site sequence abstracted from myoglobin, we evaluated this design strategy for both natural and non-natural reactivity. Polymerization stabilizes conserved structural motifs through backbone-enforced secondary structure and preserved coordination environments. Whereas the monomer exhibits unstable monohistidine ligation, the polymer enforces a stable bis-histidine coordination geometry. This structural enforcement produces a ~250 mV decrease in redox potential relative to the free monomer, indicating a substantial alteration of the heme electronic environment. In contrast to the monomer, the polymer also stabilizes small-molecule binding, as evidenced by CO coordination. Functional evaluation of carbene insertion catalysis reveals enhanced reactivity in both the monomer and polymer relative to native myoglobin, motivating further analysis of the structural features governing enzyme-like reactivity. Importantly, polymerization homogeneously localizes multiple discrete active sites, producing non-Nernstian electrochemical behavior consistent with interacting redox centers.[6,7] This multivalent organization mimics features of multimeric hemoproteins and enables cooperative electronic effects absent in the monomeric peptide. Through polymer-induced control over steric and hydrophobic environments, this platform compensates for the absence of the native protein matrix while spatially organizing redox centers within a tunable synthetic scaffold. The resulting ELPs preserve enzyme-like active-site electronics, enhance stability and catalytic performance, and establish a scalable framework for constructing multimeric hemoprotein mimetics capable of both biological and abiological function.

REFERENCES

1. Coelho, P. S.; Brustad, E. M.; Kannan, A.; Arnold, F. H. Olefin Cyclopropanation via Carbene Transfer Catalyzed by Engineered Cytochrome P450 Enzymes. *Science* **2013**, *339* (6117), 307–310.
2. Hou, K.; Huang, W.; Qi, M.; Tugwell, T. H.; Alturaifi, T. M.; Chen, Y.; Zhang, X.; Lu, L.; Mann, S. I.; Liu, P.; Yang, Y.; DeGrado, W. F. De Novo Design of Porphyrin-Containing Proteins as Efficient and Stereoselective Catalysts. *Science* **2025**, *388* (6747), 665–670. https://doi.org/10.1126/science.adt7268.
3. Leone, L.; Chino, M.; Nastri, F.; Maglio, O.; Pavone, V.; Lombardi, A. Mimochrome, a Metalloporphyrin-Based Catalytic Swiss Knife. *Biotechnol. Appl. Biochem.* **2020**, *67* (4), 495–515.
4. Reedy, C. J.; Gibney, B. R. Heme Protein Assemblies. *Chem. Rev.* **2004**, *104* (2), 617–650.
5. Oktawiec, J.; M. Ebrahim, O.; Chen, Y.; Su, K.; Sharpe, C.; D. Rosenmann, N.; Barbut, C.; J. Weigand, S.; P. Thompson, M.; Byrnes, J.; Qiao, B.; C. Gianneschi, N. Conformational Modulation and Polymerization-Induced Folding of Proteomimetic Peptide Brush Polymers. **2024**. https://doi.org/10.1039/D4SC03420A.
6. Taboy, C. H.; Bonaventura, C.; Crumbliss, A. L. Anaerobic Oxidations of Myoglobin and Hemoglobin by Spectroelectrochemistry. In *Methods in Enzymology*; Elsevier, 2002; Vol. 353, pp 187–209.
7. Robertson, D. E.; Farid, R. S.; Moser, C. C.; Urbauer, J. L.; Mulholland, S. E.; Pidikiti, R.; Lear, J. D.; Wand, A. J.; DeGrado, W. F.; Dutton, P. L. Design and Synthesis of Multi-Haem Proteins. *Nature* **1994**, *368* (6470).

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Efficient green energy production using chiral coating

Yossi Paltiel*

*Applied Physics Department, Center for Nano science and Nano technology, The Hebrew University, Jerusalem, Israel 919041 – *web: https://www.qnelab.com, e-mail: paltiel@mail.huji.ac.il*

Many biological molecules are chiral and therefore cannot be superimposed on their mirror images. Examples include amino acids and proteins, which have L chirality, and sugars, which have D chirality. This is not trivial; standard chemistry is usually symmetric with respect to both mirror images. Thermodynamics teaches us that maintaining chirality requires energy; hence, the function of chirality must entail an evolutionary advantage.
We have found that the chiral-induced spin-selective effect (CISS) [1, 2] relates electron spin and chirality, and therefore may address the above question. The same processes can be used to increase the use of green energy by enhancing production efficiency and selectivity. The CISS effect enables spin-selective current in electrolyzers, fuel cells, batteries, and solar cells. Studies conducted by our groups have demonstrated that coating the electrolyzer electrodes with chiral materials increases hydrogen production efficiency by more than 30% [3-4]. Moreover. Preliminary studies on batteries show a 15% improvement in Li-ion battery technology [5]. Lastly, the effect may enhance solar cell efficiency by enhancing the charge separation, without the need for doping [6].

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REFERENCES

1. Ron Naaman, Yossi Paltiel, David H. Waldeck; Chiral molecules and the electron spin; *Nature Review Chemistry* 3, 250–260 (2019) DOI: 10.1038/s41570-019-0087-1 (2019).
2. Brian P. Bloom,* Yossi Paltiel,* Ron Naaman,* and David H. Waldeck*, Chiral Induced Spin Selectivity, *Chem. Rev* 124, 4, 1950–1991 (2024).
3. W. Mtangi, F. Tassinari, K. Vankayala, A. V. Jentzsch, B. Adelizzi, A. R.A. Palmans, C. Fontanesi, E.W. Meijer, R. Naaman, Control of Electrons' Spin Eliminates Hydrogen Peroxide Formation During Water Splitting, *JACS* 139, 2794–2798 (2017).
4. Deb Bhowmick, Nir Yuran, Michael Fadeev, Shira Yochelis, Yossi Paltiel and Ron Naaman, Chiral metal coating to enhance water electrolysis, *Journal: Energy & Fuels* (2024). https://doi.org/10.1021/acs.energyfuels.4c04304
5. Nir Yuran, Bagavathi Muniyandi, Shira Yochelis, Daniel Sharon*, Yossi Paltiel*, Malachi Noked*; Chiral molecular coating of LiNi0.8Co0.1Mn0.1O2 cathode for high-rate capability lithium-ion batteries, *J. Phys. Chem. Lett.*, 15, 2682-2689 (2024).
6. Gur Aminadav, Omer Shoseyov, Shylee Belsey, Daniel Voignac, Shira Yochelis, Yael Levi-Kalisman, Binghai Yan, Oded Shoseyov, and Yossi Paltiel, Chiral Nematic Cellulose Nanocrystal Films for Enhanced Charge Separation and Quantum-Confined Stark Effect, *ACS nano*, 18, 42, 28609–28621 (2024).

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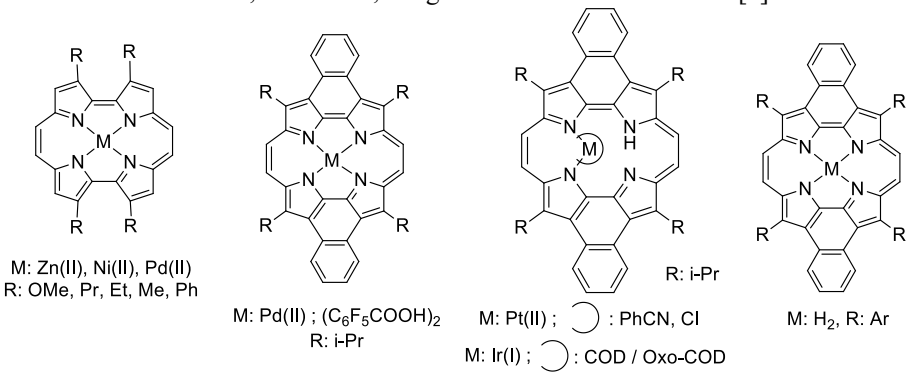
Design and Synthesis of 3,6,13,16-Substituted Porphycenes & Complexation studies of β,β'-bipyrrole fused Porphycenes

Anup Rana, J. Nagamaiah, Sameeta Sahoo, K. Narmada, K. Jiji, R. Raghuvaran, Pankaj Kumari, Arnab Dutta, Akshat Bisht, Pradeepta K. Panda

School of Chemistry, University of Hyderabad, Hyderabad – 500 046

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Porphycene is the first constitutional isomer of porphyrin and found to be more sensitive to the effect of substituents at its periphery compared to its parent isomer owing to the presence of two bipyrrolic moieties.[1] The synthetic difficulties associated with the preparation of bipyrroles limited the synthesis of porphycenes and in particular, the 3,6,13,16-substituted analogues didn't see light till 2020. We first employed the reductive dehalogenation approach to realize the first member of this series as 3,6,13,16-tetramethoxyporphycene and subsequently, we developed a rational approach to synthesize the alkyl and aryl analogues.[2]
Separately, we found β,β′-bipyrrole fusion can result not only unusual out-of-plane *cis*-bimetallic and monometallic complexation, but also in-plane complexation using palladium(II) and platinum(II) salts.[3] This led us to explore the effect of substituents, metal ions, coligands and solvents in details.[4]



REFERENCES

1. (a) Vogel, E.; Köcher, M.; Schmickler, H.; Lex, J. *Angew. Chem., Int. Ed. Engl.* **1986**, *25*, 257. (b) Sessler, J. L.; Weghorn, S. J. in Expanded, Contracted and Isomeric Porphyrins, Elsevier, Oxford, 1997. (c) Sessler, J. L.; Gebauer, A.; Vogel, E. in The Porphyrin Handbook 2000, 2, 3.
2. (a) Rana, A.; Panda, P. K. *Chem. Comm.* **2015**, *51*, 12239. (b) Rana, A.; Kumar, B. S.; Panda, P. K. *Org. Lett.* **2020**, *22*, 7175. (c) Nagamaiah, J.; Dutta, A.; Pati, N. N.; Sahoo, S.; Soman, R.; Panda, P. K. *J. Org. Chem.* **2022**, *87*, 2721. (d) Nagamaiah, J.; Dutta, A.; Sahoo, S. S.; Sahoo, S.; Panda, P. K. *New J. Chem.* **2022**, *46*, 14586. (e) Unpublished results.
3. (a) Sarma, T.; Kumar, B. S.; Panda, P. K. *Angew. Chem. Int. Ed.* **2015**, *54*, 14835. (b) Sarma, T.; Kumar, B. S.; Panda, P. K. *Chem. Rev.* **2017**, *117*, 2785. (c) Sahoo, S.; Panda, P. K. *Inorganica Chim. Acta* **2022**, *530,* 120679. (d) Sahoo, S.; Panda, P. K. *Inorg. Chem.* **2022,** *61*, 2707.
4. (a) Sahoo, S.; Sahoo, S. S.; Nagamaiah, J.; Rana, A.; Panda, P. K. *Inorg. Chem.* **2023,** *62*, 21443-21450. (b) Sahoo, S.; Kumari, P.; Panda, P. K. *J. Porphyrins Phthalocyanines* **2025**, *29*, 200-205. (c) Panda, P. K. Unpublished results.

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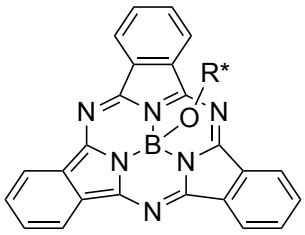


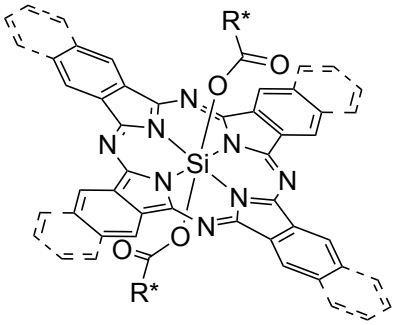
Subphthalocyanines, Phthalocyanines and Naphthalocyanines in Chiral Emissive Thin Films

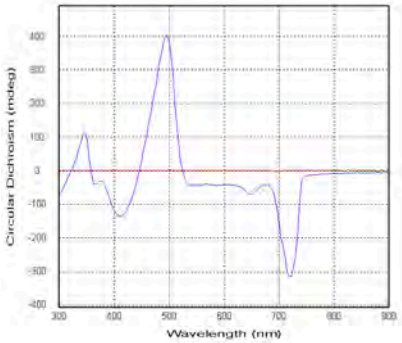
Oliver Nedderman,[a] Tiberiu M. Gianga,[b] Giuliano Siligardi,[b] G. Dan Pantoș[a]

[a] *University of Bath, Department of Chemistry, Bath BA2 7AY, UK*
[b]*University Affiliation*

Chiral silicon phtalocyanines[1] and naphthalocyanines have been used as dopants in the fabrication of chiral emissive thin films using either F8BT or F8 as polymer substrates. The point chirality of the axial ligand of the silicon phthalocyanes, leads to strong ellipticities observed on the phthalocyanine Q-band. These chiral (sub- and na-)phthalocyanines have been used in mixtures F8 or F8BT (10-30% w/w dopants) to produce chiral thin films via spincoating on fused silica plates. The film chirality has been investigated using benchtop spectrophotometers and CDi mapping in order assess their homogeneity.[2] Mueller matrix polarimetry[3] has been used to dissect the contribution of linear dichroism and birefringence as well as circular birefringence and true circular dichroism in the observed response on conventional bench-top CD spectropolarimeters. The nature / size of the axial ligand and the solvent used to manufacture the thin films influence the chiroptical properties of these films. The F8BT and F8 films are emissive and display circular polarised luminescence with a large dissimetry factor comparable with some of the best examples in the literature[4].







REFERENCES

1. "Chiral phthalocyanines through axial co-ordination" D. M. Răsădean, T. M. Gianga, A. H. Swann, G. Kociok-Köhn, **G. D. Pantoș**, *Org. Lett.* **2018,** *20*, 2645 - 2648
2. "Mapping the chiroptical properties of local domains in thin films of chiral silicon phthalocyanines by CD imaging" D. M. Răsădean, T. M. Gianga, T. Jávorfi, R. Hussain, G. Siligardi, **G. D. Pantoș**, *Molecules* **2020**, *25*, 6048
3. "Mueller Matrix Polarimetry on cyanine dye *J*-aggregates" S. R. Clowes, D. M. Răsădean, T. M. Gianga, T. Jávorfi, R. Hussain, G. Siligardi, G. D. Pantoș, *Molecules* **2023**, *28, 1523*
4. "Enantiopure synthesis of [5]helicene based molecular lemniscates and their use in chiroptical materials" L. E. M. White, T.-M. Gianga, F. Pradaux-Caggiano, C. Faverio, A. Taddeucci, H. S. Rzepa, C. Jonhannesen, L. E. Hatcher, G. Siligardi, D. R. Carbery, G. D. Pantoș, *Nat. Commun.* **2025**, 16, *2837*

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β-Alkyl-oxocorroles: Novel members of the corrinoid family

Giuseppe Pomarico[a], Martina Marsotto[b], Sara Nardis[b], Francesco Pizzoli[b], Frank R. Fronczek[c], Kevin M. Smith[c], Roberto Paolesse[b]

[a]Department of Chemistry, Sapienza - University of Rome, Piazzale Aldo Moro, 5, 00185 Rome, Italy.
[b]Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica, 1 - 00133 Rome, Italy. e-mail: roberto.paolesse@uniroma2.it
[c]Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA

ORALS

Corrole is one of the first porphyrin analogs reported in the literature, as a result of Johnson and Kay's attempt to synthesize the corrin carbon skeleton [1]. This approach was unsuccessful, and the chemistry of corrole was only sporadically explored until the new century, when the discovery of simple synthetic approaches for the preparation of 5,10,15-triarylcorroles [2] made this macrocycle available for more detailed characterization. This synthetic availability has allowed investigators to uncover important insights into the chemistry of this macrocycle, which evidences its intriguing and peculiar coordination chemistry, impressive photophysical properties, and interesting catalytic behavior. The functionalization chemistry of triarylcorroles has also been studied in detail, revealing unexpected regioselectivity and opening the way for the preparation of sophisticated molecular architectures based on corrole derivatives, with a versatility comparable to that of the parent porphyrin macrocycles. On the other hand, the chemistry of ββ-alkylcorroles has remained largely in the shadows, with very few investigations reported in the literature. In the last few years, the oxidation of 5,15-diarylcorroles at the *meso*-free position has been reported, leading to the formation of the antiaromatic 10-oxocorrole [3].
We observed the formation of 5- and 10-oxocorroles when we attempted to synthesize the Zn complexes of the corresponding corrole [4]. This reactivity led us to explore the scope of oxidation of the β-alkylcorroles, observing that this functionalization occurs under varying conditions, yielding a novel family of corrole analogs.

REFERENCES

1. Johnson AW, Kay IT. *J. Chem. Soc. (C)* 1965; 1620.
2. a) Paolesse R, Jaquinod L, Nurco DJ, Mini S, Sagone F, Boschi T and Smith KM. *Chem. Commun.* 1999; 1307. b) Gross Z, Galili N and Saltsman I. *Angew. Chem., Int. Ed. Engl.* 1999; **38**: 1427. c) Koszarna B and Gryko D. *J. Org. Chem.* 2006; **71**: 3707.
3. Ueta K, Kim J, Ooi S, Oh J, Shin J, Nakai A, Lim M, Tanaka T, Kim D, Osuka A. *J. Am. Chem. Soc.*, 2021; **143**: 7958.
4. Di Zazzo L, Nardis S, Caroleo F, Pizzoli F, Fronczek FR, Smith KM, Berionni Berna B and Paolesse R. *Chem. Commun.* 2024; **60**: 102.

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Phosphorescent porphyrin (nano)probes for sensing, imaging and cell analysis

Dmitri B. Papkovsky

School of Biochemistry and Cell Biology, University College Cork, Ireland

Phosphorescent Pt(II)-porphyrins and related structures are actively used for monitoring functional characteristics of live mammalian cells and micro-tissue models, particularly via sensing and imaging of O_2. For that, phosphorescent reporter moiety (tetrapyrrole) is functionalised or embedded in a nanoparticle structure, thus ensuring targeted delivery, usable sensing properties of the resulting probe and its ability to perform the desired analytical task(s) [1]. Still, the library of such probes is rather limited.

Here, we present several new types of such probes and sensing applications, namely:

- The small molecule O_2 probes comprising heterofunctional derivatives of Pt-pentafluorophenylporphine (PtPFPP) with tuneable hydrophilicity and cell penetration, optimised for sensing and imaging of cell and tissue O_2 [2];
- Intravital cell-penetrating probe(s) comprising core-shell nanoparticles of a biocompatible amphiphilic polymer (RL100 hydrogel) impregnated with Pt-benzoporphyrin dye. Such liquid probe, when injected into animal tissue or incorporated in a grafted tumour, allows monitoring of distribution and dynamics of tissue O_2 in live animals on a dedicated phosphorescence imager - for up to 15 days [3];
- New phosphorescent bio-scaffolding materials comprising Matrigel® precursor blended with the O_2 sensing nano-probe and deposited on suitable substrates. Such hybrid 3D scaffolds allow the design of advanced micro-tissue models (spheroids and organoids), with effective control of their oxygenation and metabolic state by O_2 sensing and imaging [4].

In this talk, structures and working characteristics of the bio-probes and initial experimental data produced with live cells and tissue models will be presented.

REFERENCES

1. L Li, AV Zhdanov, DB Papkovsky, Sens Actuat B, 2025, 137303.
2. C Zanetti, RDL Gaspar, et al., Bioconj Chem, 2022, 33 (11), 2161-2169.
3. AV Zhdanov, R Sen, et al., Sci Rep, 2023, 13 (1), 18732.
4. L Li, AV Zhdanov, DB Papkovsky, Sensors, 2026 (in press).

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Efficient Corrosion Protection of Aluminum Alloys Using Metallophthalocyanines for Electrochemical Applications

Jong Seung Park

School of Chemical Engineering, Department of Organic Material Science and Engineering, Pusan National University, Busan, 46241, Republic of Korea

ORALS

The corrosion instability of aluminum (Al)u alloys severely limits their deployment as current collectors and structural components in electrochemical environments, particularly at elevated temperatures and under aggressive electrolyte conditions [1-4]. Herein, we systematically investigate the corrosion-inhibition behavior of metallophthalocyanines (MPcs) using electrochemical, spectroscopic, and surface-analytical methods. Potentiodynamic polarization (PDP), electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), SEM–EDS, and XPS were employed to elucidate adsorption behavior, inhibition efficiency, and passivation mechanisms under varying concentrations, temperatures, and immersion durations.

Several selected phthalocyanines exhibited superior inhibition performance, achieving low corrosion current densities and high inhibition efficiencies under given conditions. The corresponding adsorption equilibrium constants indicate strong surface affinity and formation of a stable chemisorbed protective layer. At elevated temperature and extended immersion, the inhibitors still maintained high protection efficiencies, demonstrating high adsorption stability. Surface analyses confirmed the formation of a compact, nitrogen-rich interfacial layer suppressing anodic dissolution and cathodic hydrogen evolution, consistent with mixed-type inhibition behavior.

In the working mechanism, the corrosion protection arises from synergistic effects of (i) π-electron donation and coordination bonding between MPc nitrogen centers and Al surface atoms, (ii) planar macrocyclic surface coverage enhancing barrier properties, and (iii) stabilization of the native oxide/passivation film. The adsorption behavior follows Langmuir-type isotherm characteristics, suggesting monolayer formation with strong metal–inhibitor interaction.

This study establishes MPcs as highly efficient, low-concentration corrosion inhibitors for aluminum alloys. The current findings highlight the potential of tailored macrocyclic π-conjugated molecules for the development of corrosion-resistant electrochemical architectures.

REFERENCES

1. T. M. Tekaligne, H. K. Bezabh, S. K. Merso, K. N. Shitaw, M. A. Weret, Y. Nikodimos, S.-K. Jiang, S.-C. Yang, C.-H. Wang, S.-H. Wu, W.-N. Su, B. J. Hwang, Enhancing aluminum foil performance in aqueous and organic electrolytes: dual-secure passivation with phthalocyanine as a corrosion inhibitor. J. Mater. Chem. A 2024, 12, 2157–2171.
2. N. Nnaji, P. Sen, T. Nyokong, Aluminum corrosion retardation properties of acetamidophenoxy phthalocyanines: Effect of central metal. J. Mol. Struc. 2021, 1242, 130806.
3. C. Verma, E. E. Ebenso, M. A. Quraishi, K. Y. Rhee, Phthalocyanine, naphthalocyanine and their derivatives as corrosion inhibitors: A review. J. Mol. Liq. 2021, 334, 116441.
4. Y. W. Choi, A. A. Raheem, S. J. Park, J. M. Park, G. Lee, S. Lee, J. S. Park, Discoloration of triphenylmethane dyes in ethylene glycol-water coolant medium. J. Electrochem. Sci. Te. 2025, 16, 83-91.

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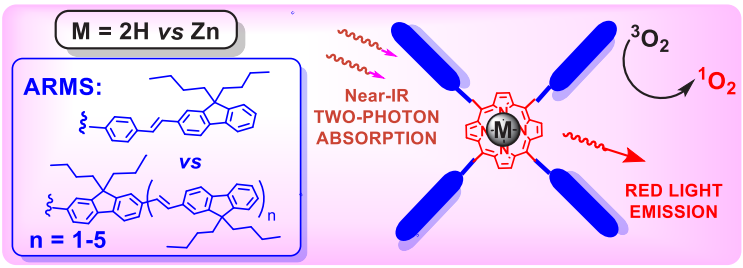


New Fluorescent Porphyrins with Fluorenyl-containing Arms Designed for Optics

Christine Paul-Roth, Frédéric Paul, Olivier Mongin

Univ Rennes, INSA Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) UMR 6226, F-35000 Rennes, France. E-mail: christine.paul@univ-rennes.fr and christine.paul@insa-rennes.fr

In 2004, we synthesised a porphyrin with four fluorenyl arms (**TFP**), which exhibited a remarkably high fluorescent quantum yield (24%) compared to the reference tetraphenylporphyrin (**TPP**), demonstrating the capacity of the fluorenyl units to enhance fluorescence.[1] Then, to exploit this efficiency, a series of Dendrimers based on **TPP** porphyrin core and bearing, in a non-conjugated way, fluorenyl dendrons was prepared.[2-4] Different applications were exploited: as the fabrication of red Organic Light Emitting Diodes (OLEDs),[5-6] and supramolecular assemblies.[7] In 2016, a family of conjugated Dendrimers, still based on **TPP,** was obtained [8]. More recently, a new family of dendrimers based on the promising **TFP**-Bu has been explored.[9]
Then, to improve light-harvesting in our dendrimers, we explored new *fluorene-based connectors*[10] and *1,4-phenyl-{carbazol or diphenylamine}-based connectors* (instead of the more classic *1,3,5-phenylene one*).[11] Later, these Dendrimers were compared with Star-shaped *meso*-substituted Porphyrins with Fluorenyl-containing Arms (n = 1-5; see Figure).[12] For these star-like porphyrins with extended fluorenyl arms, the detailed luminescence properties are discussed in the context of two-photon-induced theranostics. To improve the performance, the impact of Periphery-Conjugated Electron-Releasing Groups (diphenylamine) on optical properties is also considered.[13]



REFERENCES

[1] C. Paul-Roth, G. Williams, J. Letessier, G. Simonneaux *Tetrahedron Lett.* **2007**, 48, 4317. [2] S. Drouet, C. Paul-Roth, G. Simonneaux, *Tetrahedron* **2009**, 65, 2975. [3] S. Drouet, C. O. Paul-Roth, *Tetrahedron* **2009**, 65, 10693. [4] A. Merhi, S. Drouet, N. Kerisit, C. O. Paul-Roth, *Tetrahedron* **2013**, 69, 7112. [5] S. Drouet, C. O. Paul-Roth, V. Fattori, M. Cocchi, J. A. G. Williams, *New J. Chem.* **2011**, 35, 438. [6] X. Ren, A. Ren, J. Feng, C. Sun, *Journal of Photochemistry and Photobiology A: Chemistry* **2009**, 203, 92. [7] S. Drouet, A. Merhi, G. Argouarch, F. Paul, O. Mongin, M. Blanchard-Desce, C. O. Paul-Roth, *Tetrahedron* **2012**, 68, 98. [8] a) Yao, D.; Hugues, V.; Blanchard-Desce, M.; Mongin, O.; Paul-Roth, C. O.; Paul, F. *New J. Chem.* **2015**, 39, 7730; b) D. Yao, X. Zhang, O. Mongin, F. Paul and C. O. Paul-Roth, *Chem. Eur. J.* **2016**, 22, 5583. [9] a) D. Yao, X. Zhang, A. Triadon, N. Richy, O. Mongin, M. Blanchard-Desce, F. Paul and C. O. Paul-Roth, *Chem. Eur. J.* **2017**, 23, 2635; b) D. Yao, X. Zhang, S. Abid, L. Shi, M. Blanchard-Desce, O. Mongin, F. Paul, C. O. Paul-Roth, *New J. Chem.* **2018**, 42, 395. [10] X. Zhang, S. Ben Hassine, N. Richy, O. Mongin, M. Blanchard-Desce, F. Paul, C. O. Paul-Roth, *New J. Chem.* **2020**, 44, 4144. [11] L. Shi, Z. Sun, N. Rich, O. Mongin, M. Blanchard-Desce, F. Paul, C. O. Paul-Roth, *Photochem* **2023**, 3, 336. [12] L. Shi, Z. Sun, N. Rich, O. Mongin, M. Blanchard-Desce, F. Paul, C. O. Paul-Roth, *Chem. Eur. J.* **2024**, 30, e202303243. [13] L. Shi, S. Chi, V. Gorbunova, N. Richy, M. Blanchard-Desce, O. Mongin, F. Paul, C. O. Paul-Roth *ChemPhotoChem* **2025**, 9, e202500086.

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π-Delocalisation in 2D and 3D Conjugated Skeletons

Miłosz Pawlicki[a]

[a]*Faculty of Chemistry, Jagiellonian Univeristy, Gronostajowa 2, Kraków. Poland.*

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Strongly conjugated carbon-based systems are extensively explored in several aspects focusing on optimisation of synthetic paths and followed by understanding the properties hidden within the skeletons of different size and shape. An extended conjugation based on sp^2 hybridization of carbon allows tuning of the behaviour extracted from the number of available π-electrons eventually controlling optical and magnetic properties including a biradical character. An incorporation of a heteroatom into π-extended system is a separate possibility of modification that can be treated as a source of modulation of the optical properties. A boron involvement into those systems is a vibrant field deeply modifying the recorded properties,[1] and based on the properties of boron itself and an electron deficiency of this element that deeply disturbs the electron distribution in defected π-conjugated systems,[2,3] but also stabilizes derivatives with a paratropic character typical for antiaromatic derivatives.[4,5]

The precisely planned strategy for formation of hybrid structures linking in one skeleton acene(s) or heteroacenes modulated by a presence of a specific defect predefined for binding small cation creates strictly designed systems. It results in, depending on the complexity of the final molecule, the observation of local effects of conjugation efficiently influencing properties of each subunit. A specific construction opens a possibility for observation of the reactivity characteristic for isolated unsaturated units[6] in addition creating an opportunity for switching on the global diatropic currents[2-5] or stabilization of a biradical character.[7] All those effects will be presented and discussed focusing on the delocalization paths within precisely designed structural motifs introducing triangular defect(s) open for a post-synthetic modifications[8,9] or opening potential for a dynamic equilibrium and stabilization of open-shell character by showing the synthetic approach followed by the spectroscopic behaviour extended by XRD analysis and theoretical support.

REFERENCES

1. K. Dzieszkowski, et al. *Mater. Chem. Front.* **2022***, 6,* 3306-3311
2. W. Stawski, *et al. Angew. Chem. Int. Ed.* **2019**, *58*, 10946-10950
3. K. Bartkowski, *et al. Angew. Chem. Int. Ed.*, **2021**, *60*, 9063-9070
4. A. Dutta, et al. *Org. Lett.* **2021***, 23,* 9436-9440
5. K. Wypych, et al. *Org. Lett.* **2022***, 24,* 4876-4880
6. J. Klajn, et al. *Chem. Commun.* **2019**, *55*, 4558-4561
7. P. Banachowicz, M. Das, et al. *Angew. Chem. Int. Ed.* **2024***, 63, e202400780*
8. M. Farinone, et al. *Chem. Commun*. **2022***, 58,* 7269-7272
9. K. Dzieszkowski, et al. *Chem. Commun.* **2026**, *62*, advance article

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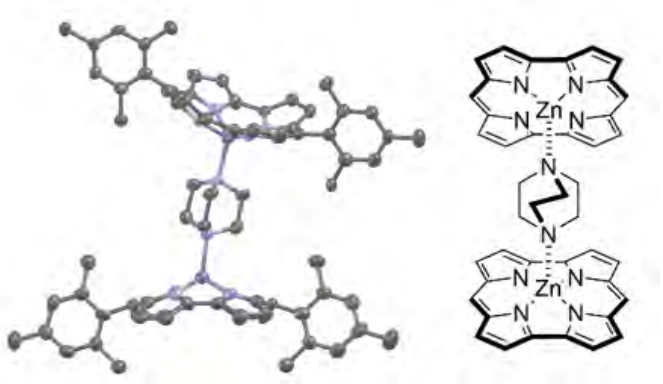


Manifestations of (anti)aromaticity in porphyrinoids big and small

Martin D. Peeks[a]

[a]*School of Chemistry, University of New South Wales, UNSW Sydney NSW 2052 AUSTRALIA*

One of the most attractive features of the concept of aromaticity is that it seems to offer a common origin for properties spanning stability, structure, magnetism, and photochemistry. By exploring the extremes of (anti)aromaticity we might evaluate to what extent chemists' "working definitions" of aromaticity compare to reality. We have recently shown, and will discuss, how aromaticity in oxidised porphyrin nanorings[1] is associated with an increase in electronic delocalization compared to rings in non-aromatic oxidation states.[2]
In the much smaller size regime, we explore the differences between aromaticity and antiaromaticity by comparing porphyrin (aromatic) and its ring-contracted sibling norcorrole,[3,4] which has a 16 π-electron circuit and is antiaromatic. We have synthesised zinc norcorrole and its supramolecular complexes.[5] Surprisingly, zinc norcorrole has almost the same ring current strength (in nA/T) to that in zinc porphyrin, albeit of opposite sign. It has approximately 100-fold higher binding constants to N-containing axial ligands (DABCO crystal structure shown in Figure) than porphyrin, likely due to the norcorrole's extreme curvature, which exposes the norcorrole's Zn^{2+} for binding.



REFERENCES

1 M. Jirásek, H. L. Anderson and M. D. Peeks, *Acc. Chem. Res.*, **2021**, *54*, 3241–3251.
2 D. Bradley, B. K. Hillier and M. D. Peeks, *Chem. Commun.*, **2023**, *59*, 13438–13441.
3 M. Bröring, S. Köhler and C. Kleeberg, *Angew. Chem. Int. Ed.*, **2008**, *47*, 5658–5660.
4 T. Ito, Y. Hayashi, S. Shimizu, J.-Y. Shin, N. Kobayashi and H. Shinokubo, *Angew. Chem. Int. Ed.*, **2012**, *51*, 8542–8545.
5 D. Bradley, R. Tian, M. Bhadbhade, L. Macreadie, C. Sarowar and M. D. Peeks, *Inorg Chem*, **2024**, DOI:10.1021/acs.inorgchem.4c01146.

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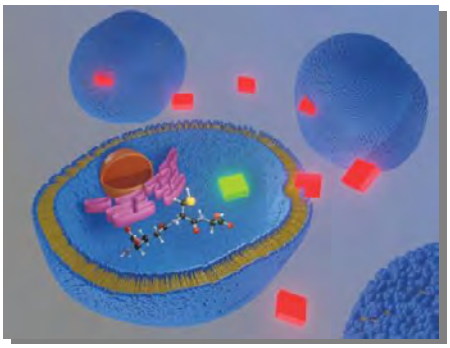
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Self-Assembly and Supramolecular Design of Functional Nanostructured Materials for Biological Interfacing

Lluïsa Pérez-García[a,b], Pascual López-Algarra[a,b], Saman Bagherpour[a,b], Alba Pereda-Velarde[c,d,e], Silvia Gines[c,d,e], Patricia Vázquez[f,g], Marta Duch[h], Juan Pablo Agusil,[h] José Antonio Plaza[h], Mariano Redondo-Horcajo[f], Teresa Suárez[f]

[a]*Departament de Farmacologia, Toxicologia i Química Terapèutica, Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, Barcelona, 08028, Spain. Email: mlperez@ub.edu*
[b]*Institut de Nanociència i Nanotecnologia IN2UB, Universitat de Barcelona, Barcelona, 08028, Spain.*
[c]*Departament de Biomedicina, Facultat de Medicina i Ciències de la Salut, Institut de Neurociències, Universitat de Barcelona, Barcelona, 08036, Spain.*
[d]*Institut d'Investigacions Biomèdiques August Pi i Sunyer (IDIBAPS), Barcelona, Spain.*
[e]*Centro de Investigación Biomédica en Red sobre Enfermedades Neurodegenerativas (CIBERNED), Madrid, Spain.*
[f]*Centro de Investigaciones Biológicas Margarita Salas, CIB (CSIC), Madrid, 28040, Spain.*
[g]*Departamento de Bioquímica y Biología Molecular, Facultad de Medicina, Universidad Complutense de Madrid, Madrid, 28040, Spain*
[h]*Instituto de Microelectrónica de Barcelona, IMB-CNM (CSIC), Campus UAB, Cerdanyola del Vallès, Barcelona, 08193, Spain.*

Controlling interactions between nanomaterials and living cells is central to advances in nanomedicine[1]. We develop chemically programmed, self-assembled and supramolecular materials—including hydrogels, nanoparticles, and silicon-based microdevices[2]—to sense, monitor, and modulate cellular behavior. These platforms enable applications in biosensing, intracellular signaling, targeted delivery, and mechanical control of individual cells.



This talk will present examples of how supramolecular chemistry enables precise control over the properties and functions of advanced nanomaterials. In particular, the functionalization of silicon microchips,through self-assembled monolayers, to enhance cellular uptake and real-time intracellular glutathione sensing will be described[3]. Also, we will discuss self-assembling BODIPY-based scaffold capable of mitochondrial targeting, highlighting its potential applications in bioimaging and drug delivery.

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References
[1] Domingues, C. et al. Where Is Nano Today and Where Is It Headed? A Review of Nanomedicine and the Dilemma of Nanotoxicology. ACS Nano 2022, 16, 9994–10041.
[2] Arjona, M.I. et al. Intracellular Mechanical Drugs Induce Cell-Cycle Altering and Cell Death. Adv. Mater. 2022, 2109581.
[3] Bagherpour, S. et al. Silicon oxide microchips functionalized with fluorescent probes for quantitative real-time glutathione sensing in living cells. J. Mater. Chem. B, 2025, 13, 1630–1642.

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Porphysome-mediated photodynamic immune stimulation

Layla Pires[a], Carla Calcada[a], Michael Valic[a], Tracy Liu[c], Juan Chen[b], Gang Zheng[b], Brian C Wilson[b]

[a] *Texas A&M University, Department of Biomedical Engineering*
[b] *University Health Network, Princess Margaret Cancer Center*
c West Virginia University

Porphysomes are biodegradable, liposome-like nanoparticles composed of porphyrin-lipid building blocks that self-assemble into vesicular structures, serving as multifunctional theranostic nanocarriers. Their unique optical properties enable applications in photoacoustic and fluorescence imaging, as well as photothermal and photodynamic therapies. Beyond direct tumor ablation, light-activated porphysomes can elicit a robust immune response, a phenomenon termed photodynamic immune stimulation. Tumor accumulation primarily occurs via the enhanced permeability and retention (EPR) effect, with radiographic studies revealing preferential localization at tumor margins, yet still achieving significant tumor damage and immune activation.

Our group has investigated porphysome-mediated therapy across multiple tumor models, including pancreatic, head and neck, melanoma, and lung cancers. Remarkably, effective immune stimulation can be achieved with light doses as low as 20 J/cm², making this approach particularly advantageous for thick or pigmented tumors where light penetration is limited. Biomarker analysis demonstrates upregulation of both innate and adaptive immune pathways, rapid neutrophil activation within hours of treatment, and recruitment of immune cells into the tumor microenvironment. Furthermore, adoptive immune transfer experiments confirm the establishment of immune memory, as naïve mice receiving splenocytes from treated donors exhibit controlled tumor growth. These findings highlight porphysomes as a promising platform for synergistic photodynamic therapy and immunotherapy, offering a pathway toward durable cancer control.

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Displacement of Methionine Coordination at the Heme Iron in Regulation of Signaling and Redox Pathways

Ekaterina Pletneva[a]

[a]*Department of Chemistry, Dartmouth College, Hanover, New Hampshire, USA*

ORALS

Ligand substitution at the heme iron takes place in many signaling pathways and is broadly relevant in regulation of electron transfer. Substitution or loss of the Met coordination are common. In our studies of native and engineered cytochromes (cyt), we examine factors that pose Met for displacement at the heme iron and describe associated changes in conformational and redox properties of these proteins. The replacement of Met80 by a Lys residue in mitochondrial cyt *c* typically takes place at high, alkaline, pH. However, disease mutations and interactions with cardiolipin-rich membranes shift this transition to lower pH values. The effects stem from destabilization of the protein structure. Our analyses of cyt *c* variants revealed the importance of the hydrogen-bonding network and the foldon hierarchy in propagation of structural changes. For mutants having Thr49 and/or Thr78 substituted by a Val, the extent of destabilization is similar for the ferric and ferrous Met-ligated conformers, but the ligation outcome differs because the global stability of the protein and stabilities of its foldons depend on the redox state of the heme iron. Replacement of Met by NO is relevant for bacterial proteins in low-oxygen environments when oxygen reduction and denitrification pathways may coexist. Our studies of diheme cytochromes have identified that interface interactions and domain-swapped architecture in these proteins underline the integrity of the Met coordination to the heme iron.

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Synthesis and Spectroscopy of Hypervalent P(V) and Sb(V) Porphyrins with Charge Transfer NIR Transitions

Prashanth K. Poddutoori,[a] Peyton Ellis,[a] Abby Kothman,[a] Jam R. Hamza,[a] Jatan K. Sharma,[b] Paul A. Karr,[c] Art van der Est,[d] Francis D'Souza[b]

[a]*Department of Chemistry & Biochemistry, 1038 University Drive, University of Minnesota Duluth, Duluth, MN, 55812, USA. Email: ppk@d.umn.edu*
[b]*Department of Chemistry, University of North Texas, 1155 Union Circle, # 305070, Denton, Texas 76203-5017, USA.*
[c]*Department of Physical Sciences and Mathematics, Wayne State College, 1111 Main Street, Wayne, Nebraska 68787, USA.*
[d]*Department of Chemistry, 1812 Sir Isaac Brock Way, Brock University, St. Catharines, ON, L2S 3A1, Canada.*

Phosphorus(V) and antimony(V) porphyrins possess unique axial-bonding capabilities, along with rich redox and optical properties, which distinguish them from other main-group and transition-metal porphyrins. These features make them promising candidates for applications in solar energy harvesting, molecular electronics, catalysis, and biomedicine. Despite their potential, Group 15 porphyrins remain underexplored. In this context, our research group focuses on hypervalent Group 15 porphyrins. Over the past few years, we have investigated push–pull-type hypervalent Group 15 porphyrins that exhibit intramolecular charge transfer (ICT). Incorporation of P(V) or Sb(V) ions into the porphyrin cavity generates a highly electron-deficient core; when electron-rich substituents are present at the meso positions, efficient ICT is induced. Recently, we expanded this strategy to a range of tetraarylporphyrins bearing strong electron-donating meso substituents such as trimethoxyphenyl, triphenylamine, dimethylaniline, and ferrocene.[1-4] Upon metalation with P(V) or Sb(V), the resulting hypervalent porphyrins display pronounced ICT from the meso substituents to the central porphyrin ring. The extent of ICT strongly depends on the donating strength of the meso substituent, with the strongest effect observed in ferrocene-containing porphyrins. This behavior is reflected in their optical and emissive properties, as their absorption bands are significantly red-shifted into the near-infrared region and exhibit high molar extinction coefficients. Remarkably, some of these porphyrins exhibit CT character in their emission that originates from the singlet and triplet excited states. In this presentation, I will discuss the synthesis, structures, redox behavior, and remarkable photophysical properties of these porphyrins.

REFERENCES

1. Hamza, J. R.; Sharma, J.; Karr, P. A.; van der Est, A.; D'Souza, F.; Poddutoori, P. K. *J. Am. Chem. Soc.*, **2024**, *146*, 25403.
2. Holzer, N.; Sharma, J.; D'Souza, F.; Poddutoori, P. K. *ACS Omega*, **2024**, *9*, 22892.
3. Zarrabi, N.; Sharma, J. K.; Andzelevich, K.; Karr, P. A.; van der Est, A.; D'Souza, F.; Poddutoori, P. K. *Inorg. Chem.* **2025**, *64*, 8958.
4. Poddutoori, P. K. *Dalton Trans*. **2023**, *52*, 14287.

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Ag(III) β-alkylcorrolates: the simple made complex

Giuseppe Pomarico[a], Martina Marsotto[b], Manuela Stefanelli[b], Frank R. Fronczek[c], Roberto Paolesse[b]

[a]*Department of Chemistry, Sapienza - University of Rome, Piazzale Aldo Moro, 5 - 00185 Rome, Italy. e-mail: giuseppe.pomarico@uniroma1.it*
[b]*Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica, 1 - 00133 Rome, Italy.*
[c]*Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA*

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Among coinage metal corrole complexes, silver reprents an intriguing case, as Ag-arylcorrolates can exhibit either innocent (similarly to gold complex) or noninnocent (as copper) behavior, depending on the substituition pattern (and geometry) of the macrocycle [1]. Furthermore, the coordinated metal significantly dictates the optical and electronic properties of the macrocycle, as well as its reactivity.
For instance the silver complex of triarylcorrole displays a regioselectivity toward nitration [2] or bromination [3] that is not observed in either the Cu analogue or the free base corrole.
However the behavior of the Ag complexes of the electron-rich β-alkylcorroles is unknown. For this reason, we attempted the synthesis of the corresponding silver complexes. The coordination reaction proved challenging, as the outcome was highly sensitive to both the choice of solvent and the silver(I) source. Notably, complex formation is frequently accompanied by the facile functionalization at the free *meso* positions, alongside the formation of oxidation by-products as oxocorroles [4]. While initially problematic, this reactivity may offer significant synthetic utility, enabling the one-pot preparation of diversely functionalized macrocycles.

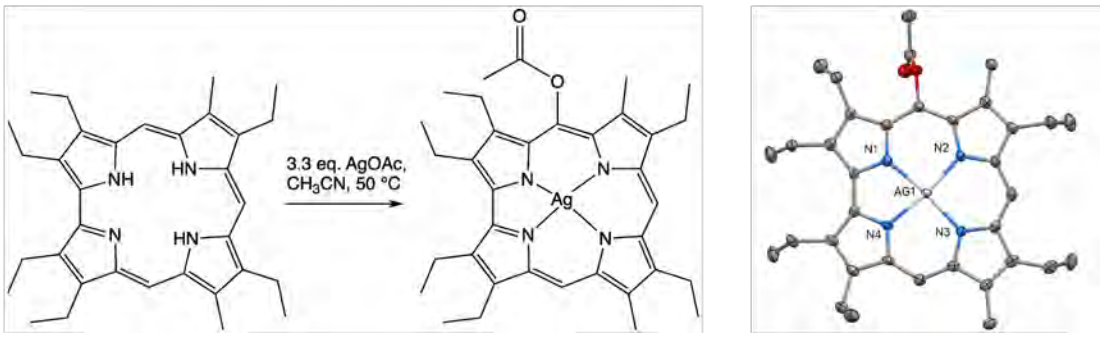


Figure 1. One of the products obtained by alkylcorrole metalation with Ag(I) salt.

REFERENCES

1. K. E. Thomas, H. Vazquez-Lima, Y. Fang, Y. Song, K. J. Gagnon, C. M. Beavers, K. M. Kadish, A. Ghosh. *Chem. Eur. J.* **2015**, *21*, 16839 – 16847.
2. M. Stefanelli, M. Mastroianni, S. Nardis, S. Licoccia, F. R. Fronczek, K. M. Smith, W. Zhu, Z. Ou, K. M. Kadish, R. Paolesse. *Inorg. Chem.* **2007**, *46*, 10791 – 10799.
3. M. Stefanelli, M. L. Naitana, M. Chiarini, S. Nardis, A. Ricci, F. R. Fronczek, C. Lo Sterzo, K. M. Smith, R. Paolesse *Eur. J. Org. Chem.* **2015**, 6811 – 6816.
4. L. Di Zazzo, S. Nardis, F. Caroleo, F. Pizzoli, F. R. Fronczek, K. M. Smith, B. Berionni Berna, R. Paolesse. *Chem. Commun.* **2024**, *60*, 102.

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Langmuir Monolayers as a Platform for Scalable Two-Dimensional Photocatalytic Membranes

Sarah Jasmin Finkelmeyer[a], Konrad Hotzel[b], Charlotte Mankel[b], Stefan Zechel[b,c,e,f], Martin D. Hager[b,c,d,e,f], Ulrich S. Schubert[b,c,d,e,f], Kalina Peneva[b,c,d], Martin Presselt[a,d]

[a] *Leibniz Institute of Photonic Technology (IPHT), Jena, Germany*
[b] *Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University Jena, Jena, Germany*
[c] *Jena Center for Soft Matter (JCSM), Friedrich-Schiller-University Jena, Jena, Germany*
[d] *Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany*
[e] *Helmholtz Institute for Polymers in Energy Application Jena (HIPOLE Jena), Jena, Germany*
[f] *Helmholtz Zentrum Berlin für Materialien und Energie (HZB), Berlin, Germany*

Langmuir-Blodgett (LB) layers[1] are ideal platforms for developing photocatalytic membranes composed of uniformly aligned[2] charge-transfer units. Matrix amphiphiles in the LB layer support alignment,[3] enable fine-tuning of energy levels[4] and accommodate catalysts and photosensitizers, such as porphyrins and phthalocyanins. This architecture enables the coupling of oxidation and reduction to opposite sides of a molecular membrane.

We focus on the photo-catalytic hydrogen evolution reaction. To increase catalyst loading per volume, we employ a spiral-wound configuration that accommodates large membrane areas within a single GC vial (Figure 1(a)). Embedding the catalyst in the LB membrane yields turnover numbers that exceed those achieved under homogeneous conditions (Figure 1(c)). This highlights the applicability of two-dimensional membranes in photocatalysis.

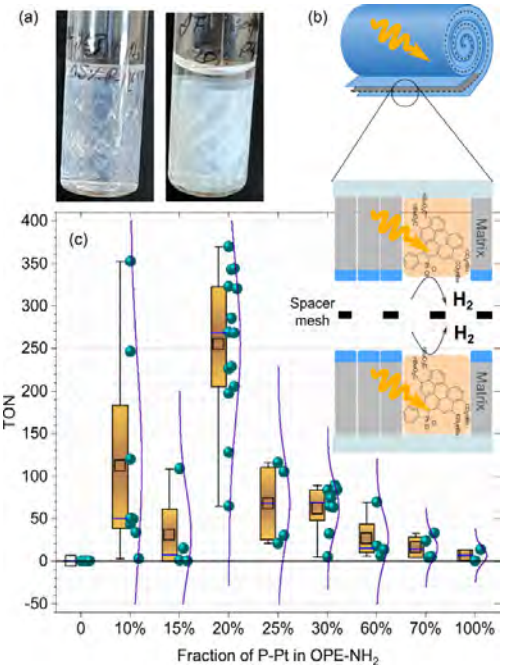


Figure 1. Spiral wound configuration of a layer system containing a two-dimensional catalytic membrane. (a) samples in GC-vial, (b) schematic representation, and (c) TON from hydrogen evolution.

REFERENCES

1. M. L. Hupfer, B. Dietzek-Ivansic, M. Presselt, et al., *Advanced Materials* **2023**, *35*, e2204874
2. M. L. Hupfer, W. Dehaen, M. Presselt, et al., *Advanced Materials Interfaces* **2021**, *9* (1), 2101490
3. S. J. Finkelmeyer, M. Presselt, *Chemistry – A European Journal* **2025**, *31*, e202403500
4. S. J. Finkelmeyer, K. Glusac, F. H. Schacher, M. Presselt, et al., *Advanced Materials* **2023**, *5*, e2305006

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Understanding the steric influence in α-substituted metal phthalocyanines on synthesis, structure and reactivity

Sebastian Pätsch[a], Aleksandr Penni[a], Luis A. Gallego-Villada[b], Dmitry Yu. Murzin[b], Päivi Mäki-Arvela[b], Alexander Efimov[a]

[a]*Tampere University, Chemistry and Advanced Materials, 33720 Tampere, Finland*
[b]*Åbo Akademi University, Industrial Chemistry and Reaction Engineering, 20500 Turku, Finland*

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The potential of metal phthalocyanines (MPc) in catalytic application is well established in the common literature, to a large extent because of their structural relationship to biological porphyrin systems. For the most part, catalytically active 1st row transition metals (e.g. Co, Fe, Cu, Zn) are employed for prepation of homogeneous catalysts which represent cost-efficient and easy accessible compounds. Nevertheless, phthalocyanines and their metal complexes need modification of the isoindole backbone to circumvent the two major drawbacks of phthalocyanines for homogeneous catalysis: bad solubility and aggregation. Heterogenization of MPcs (on e.g. zeolites) represents an alternative pathway to expand the applicability. In addition, it also enables studies in polar, protic solvents or even gas phase reactions. [1]

Our group introduced non-aggregating α-substituted tetrakis[3,5-(di-*tert*-butyl)phenyl] phthalocyanines which are readily synthesized from the corresponding phthalonitrile via the lithium/1-octanol route.[2] Alternatively, these phthalocyanines are also accessible from magnesium alkoxides or by base-catalyzed direct metalation in 1-pentanol. Interestingly, the isomeric mixture varies significantly between the different preparation methods. The lithium route serves as a selective synthesis of the C_{4h} isomer (name: windmill), whereas the alternative routes produce additionally the C_{2v} (name: frog) and C_S (name: dragon) isomers in appropriate yields and isomerically pure. In subsequent steps, the metal of choice can be inserted into the phthalocyanine ligand to enable the isolation of various new 1st, 2nd and 3rd row transition metal phthalocyanines. The non-aggregating properties of these systems were not only confirmed by spectroscopic methods (UV/vis, NMR) but also with elucidation of the molecular structure and the crystal packing by single crystal X-ray diffraction.

To our surprise, the $FePc^{windmill}$ seemed unaccessible although iron phthalocyanine chemistry is well established in the literature and contains several readily accessible examples of substituted FePcs.[3] In some cases, FePcs can dimerize under the influence of dioxygen to form the μ-oxido bridged dimer as a *resting state*.[4] However, the steric hindrance of the bulky α-substituents prohibits the dimerization in our case which leads to decomposition of the $FePc^{windmill}$. Therefore, we investigated the stability of $FePc^{windmill}$ and its derivatives and supported these findings with theoretical calculations. In addition, the results were compared with other, more stable FePcs.

Lastly, heterogenized $MPcs^{windmill}$ in zeolites were investigated for the application in catalytic methane to methanol conversion under aqueous conditions. Shifting from microporous to mesoporous material enabled the MPc for better penetration of the pores and, as a result, a better surface coverage. Additionally, the α-substituents at the isoindole backbone create a spacer between the MPc units which guarantees a mononuclear reaction site. This brings the overall system closer to a real single-atom catalyst.

REFERENCES

1. Sorokin, *Chem. Rev.* **2013**, 113, 8152
2. Tkachenko *et al.*, *Phys. Chem. Chem. Phys.* **2024**, 26, 18113
3. Metz *et al.*, *Inorg. Chem.* **1984**, 23, 1065 ; Scott *et al.*, *Fuel* **2019**, 242, 573, Eberhardt *et al.*, *Snthesis* **1997**, 95
4. Mekhryakova *et al.*, *Russ. J. Gen. Chem.* **2001**, 71, 570; Ercolani *et al.*, *Inorg. Chem.* **1983**, 22, 2584

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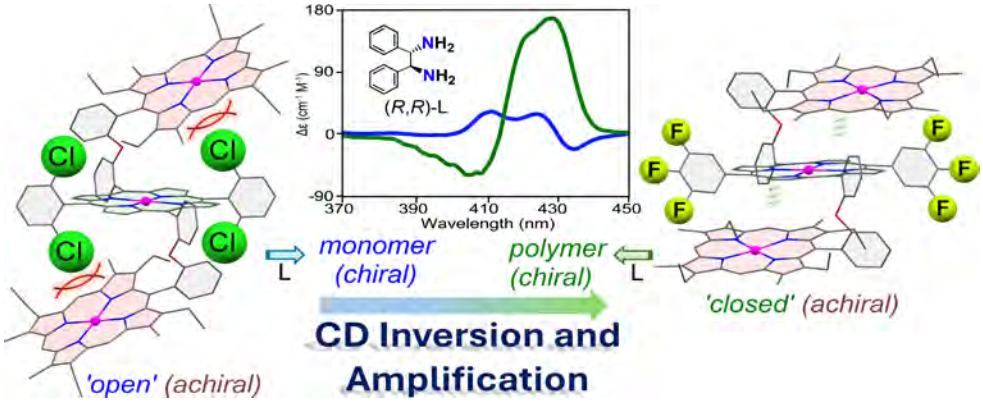
Modulation of Supramolecular Chirality using '*Nano-size*' Trizinc(II)porphyrin Trimers: A Structure-Function Correlation

S. P. Rath

Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur-208016, India

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Supramolecular chirogenesis is one of the most important interdisciplinary fields to investigate because of its occurrence in many natural and artificial systems. A complete understanding of the origin of chirality-transfer information at the electronic and molecular levels would help us determine the absolute configuration of natural products and synthetic compounds. Step-wise induction, amplification, and inversion, and reduction of molecular chirality have been achieved in a single molecular framework through successive coordination of chiral diamines to a 'nano-size' achiral trizinc(II)porphyrin trimer host, due to changes in interporphyrin interactions and helicity. Also, a subtle modification in trizinc(II) porphyrin trimer profoundly affects its complexation and chirogenic responses with chiral diamine substrates: while the 'open' form generates a 'monomeric' complex with low CD amplitude, the 'closed' form produces an exclusive 'polymer' with a large, amplified CD signal with opposite sign [1-3].



REFERENCES

1. (a) D. Chandel, G. Pescitelli, S. P. Rath *Chem. Eur. J.* **2026**, *32*, e202404425. (b) D. Chandel, C. Pal, S. P. Rath *Chem. Eur. J.* **2025**, *31*, e202404425. (c) B. Saha, C. Pal, S. P. Rath *Chem. Eur. J.* **2024**, *30*, e202402536. (d) A. Dhamija, D. Chandel, S. P. Rath *Chem. Sci.* **2023**, *14*, 6032. (e) B. Saha, S. P. Rath *Inorg. Chem.* **2022**, *62*, 2154. (f) A. Dhamija, S. P. Rath *Inorg. Chem.* **2020**, *59*, 801. (g) A. Dhamija, S. P. Rath *Inorg. Chem.* **2017**, *56*, 15203. (h) S. A. Ikbal, S. P. Rath, *J. Org. Chem.* **2016**, *81*, 5440. (i) A. Dhamija, S. P. Rath *Inorg. Chem.* **2016**, *55*, 13014.
2. (a) B. Saha, S. P. Rath *Inorg. Chem.* **2020**, *59*, 7795. (b) B. Saha, A. G. Petrovic, A. Dhamija, N. Berova, S. P. Rath *Inorg. Chem.* **2019**, *58*, 11420. (c) B. Saha, S. P. Rath *Inorg. Chem.* **2017**, *56*, 3849. (d) S. A. Ikbal, S. P. Rath *Chem. Commun.* **2015**, *51*, 14107. (e) S. A. Ikbal, S. P. Rath *Chem. Commun.* **2015**, *51*, 895. (f) S. A. Ikbal, S. Brahma, S. P. Rath *Chem. Commun.* **2014**, *50*, 14037.
3. (a) A. Dhamija, P. Mondal, B. Saha, S. P. Rath *Dalton Trans.* **2020**, *49*, 10679. (b) P. Mondal, S. P. Rath, *Coord. Chem. Rev.* **2020**, *405*, 213117.

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Photoactivation of BODIPY fluorescence with green light

Françisco M. Raymo

The Patricia and Philip Frost Institute for Chemistry and Molecular Science, University of Miami, 1201 Memorial Drive, Coral Gables, FL 33146-2509, United States

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Existing synthetic dyes with photoactivatable fluorescence demand ultraviolet radiation or, at best, violet light for fluorescence photoactivation [1]. Illumination of biological samples within this range of relatively short wavelengths, however, causes significant photodamage. Strategies for the photochemical generation of fluorescent products under irradiation at wavelengths longer than 500 nm with moderate power densities are urgently needed to enable live-cell imaging with negligible phototoxicity. We identified a possible structural design to satisfy these stringent irradiation requirements. Specifically, we demonstrated that illumination of a borondipyrromethene (BODIPY) chromophore in the green region of the visible spectrum cleaves an adjacent oxazine heterocycle to form a fluorescent product with emission in the red spectral window [2]. We successfully photoactivated this compound with a 561-nm laser and localized single molecules of the fluorescent product with nanometer precision under 581-nm excitation, even in the interior of live cells. Indeed, we reconstructed sub-diffraction images of the nanostructured lysosomes of the labeled cells under such unprecedented illumination conditions. Our results clearly indicate that this photochemical strategy for fluorescence photoactivation is a viable one for the realization of very-much needed photoactivatable synthetic dyes for super-resolution imaging with live-cell compatible irradiation requirements.

REFERENCES

1. Zhang, Y.; Zheng, Y.; Tomassini, A.; Singh, A. K.; Raymo, F. M. Photoactivatable fluorophores for bioimaging applications. *ACS Appl. Opt. Mater.* **2023**, *1*, 640–651.
2. Tomassini, A.; Liu, Y.; Zheng, Y.; Shahid, M. A.; Singh, A.; Singh, A. K.; Piedra, W. M.; Gong, X.; Hayter, C. E.; Singh, K. I.; Captain, B.; Sortino, S.; Zhang, Y.; Raymo, F. M. Photoactivation of BODIPY fluorescence with green light. *J. Org. Chem.* **2025**, *90*, 8214–8227.

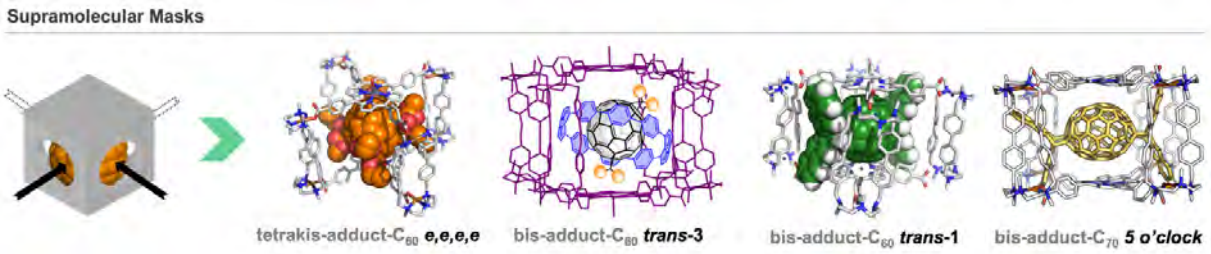
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Multipurpose Porphyrin-Based Supramolecular Nanocapsules for Chemistry at the Confined Space

Xavi Ribas[a]

[a] *Institut de Química Computacional i Catàlisi (IQCC), Universitat de Girona, E17003 Girona, Catalonia-Spain*
E-mail: xavi.ribas@udg.edu

The design of a confined cavity dictates the type of guest to be encapsulated, and supramolecular cages are tunable scaffolds that allow the rational design of their cavities. Targeting fullerenes as guests, their regioselective functionalization and the control of the number of adducts are highly important to unlock the development of fullerene chemistry. Nowadays, easy-accessible C_{60} and C_{70} fullerene mono-adducts are mainly used in any application[1] due to the hampered accessibility to pure alternative fullerene poly-adduct derivatives. In general, multi-adduct mixtures with uncontrolled regioselectivity (multi-isomers) are obtained, and chromatographic purification is too costly and time-consuming. Herein, porphyrin-based supramolecular nanocapsules[2,3] are used as supramolecular shadow masks to tame the over-reactivity of Bingel-Hirsch-type cyclopropanation reactions and, more importantly, to have full control over the equatorial regioselectivity and the number of additions. Thus, exclusively equatorial bis-, tris- and tetrakis-C_{60} adducts using ethyl-bromomalonate are stepwise obtained and fully characterized (NMR, UV-vis and XRD). Furthermore, the regioselectivity control is finely tuned using a three-shell Matryoshka-like assembly towards synthesizing a single *trans*-3 bis-Bingel-C_{60} for the first time.[4] Also, the mask strategy is extended to Diels Alder reactions with full control of the regioselectivity in the synthesis of trans-1 bis-pentacene-C_{60}.[5] These results, recently extended to C_{70},[6,7] are fully attributed to the confinement control imposed by the capsule's cavity, and represent a novel and unique strategy to infer regio-control to the synthesis of fullerene multi-adducts. We envision that the described protocol will produce a plethora of derivatives for applications such as solar cells. We will also discuss the selective purification of fullertube mixtures[8] and the encapsulation of photo-active molecular motors.[9]



REFERENCES

1. E. Castro, L. Echegoyen et al. *J. Mater. Chem. C*, **2018**, 6, 2635.
2. C. García-Simón, X. Ribas, et al. *Nat. Commun*. **2014**, 5:5557.
3. C. Fuertes-Espinosa, X. Ribas, et al, *Chem* **2020**, 6, 169–186.
4. E. Ubasart, X. Ribas, et al, *Nat. Chem*. **2021**, 13, 420-427.
5. M. Pujals, X. Ribas, et al, *Cell Rep. Phys. Sci*. **2022**, 3, 100992.
6. V. Iannace, X. Ribas et al, *J. Am. Chem. Soc*. **2024**, 146, 5186−5194.
7. T. Pèlachs, X. Ribas et al, *CCS Chem*. **2025**, 7, 703–715
8. V. Iannace, X. Ribas et al, *J. Am. Chem. Soc*. **2025**, 147, 36079−36084
9. C. Fuertes-Espinosa, X. Ribas, B. Feringa et al, *J. Am. Chem. Soc*. **2026**, 10.1021/jacs.5c16349

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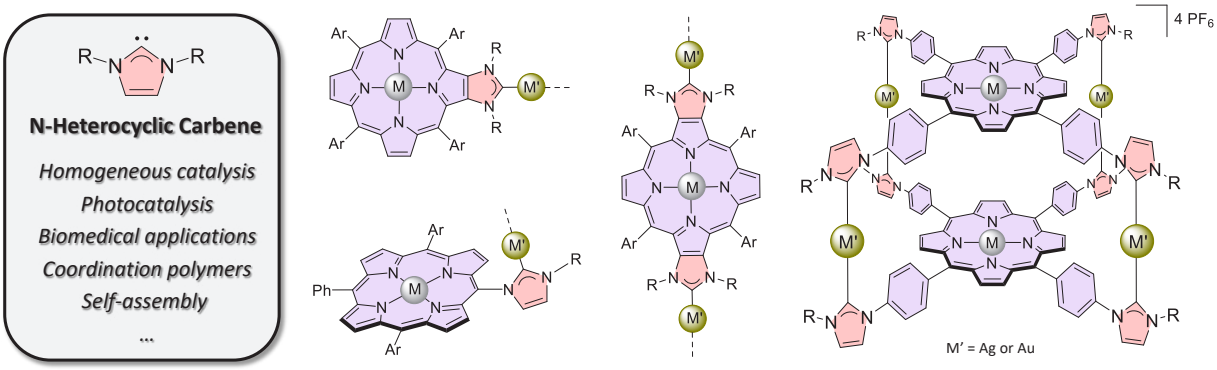
Overview of Molecular Systems Combining Porphyrins and N-Heterocyclic Carbenes and their Applications

Sébastien Richeter[a], Sébastien Clément[a], Jean-François Longevial[a], Ludivine Poyac[a], Dimitri Dessaint[a]

[a] *Institut Charles Gerhardt Montpellier, University of Montpellier, CNRS, ENSCM, Montpellier, France*

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N-heterocyclic carbenes (NHCs) are an important class of ligand in organometallic chemistry and homogeneous catalysis, attracting considerable interest from research groups specialising in these fields. Over the past 20 years, we have reported in the literature on several molecular systems in which NHC ligands are covalently linked to porphyrins [1]. We have thus demonstrated that multiporphyrin assemblies can readily be obtained from NHCs and transition metals in the form of molecular complexes [2-5] and main-chain organometallic polymers [6]. Furthermore, we have also demonstrated that the catalytic properties of these NHC ligands [7] and their corresponding metal complexes NHC-M' [8] can be affected by neighbouring porphyrins and the type of internal metal M. This presentation will therefore provide an overview of our work on this topic, as well as presenting the latest results.



REFERENCES

1. J.-F. Longevial, C. Rose, L. Poyac, S. Clément, S. Richeter, *Eur. J. Inorg. Chem.* **2021**, 776-791.
2. M. Abdelhameed, P.-L. Karsenti, A. Langlois, J.-F. Lefebvre, S. Richeter, R. Ruppert, P. D. Harvey, *Chem. Eur. J.* **2014**, *20*, 12988-13001
3. J.-F. Longevial, K. El Cheikh, D. Aggad, A. Lebrun, A. van der Lee, F. Tielens, S. Clément, A. Morère, M. Garcia, M. Gary-Bobo, S. Richeter, *Chem. Eur. J.* **2017**, *23*, 14017-14026.
4. C. Rose, A. Lebrun, S. Clément, S. Richeter, *Chem. Commun.* **2018**, *54*, 9603-9606.
5. L. Poyac, C. Rose, M. Wahiduzzaman, A. Lebrun, G. Cazals, C. H. Devillers, P. G. Yot, S. Clément, S. Richeter, *Inorg. Chem.* **2021**, *60*, 19009-19021.
6. J.-F. Longevial, M. Lo, A. Lebrun, D. Laurencin, S. Clément, S. Richeter, *Dalton Trans.* **2020**, *49*, 7005-7014.
7. J.-F. Lefebvre, M. Lo, J.-P. Gisselbrecht, O. Coulembier, S. Clément, S. Richeter, *Chem. Eur. J.* **2013**, *19*, 15652-15660.
8. L. Poyac, S. Scoditti, X. Dumail, M. Granier, S. Clément, R. Gramage-Doria, C. H. Devillers, S. Richeter, *Chem. Commun.* **2022**, *58*, 13270-13273.

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Insertion of Nitric Oxide Into a Metalloporphyrin-Carbon Bond

Tsitsi A. Kapfunde[a], Jennifer Londoño-Salazar[a], Chance Lander[a], Guan Ye[a], Yong Zhang[b], Yihan Shao[c], George B. Richter-Addo[a]

[a]*Price Family Foundation Institute of Structural Biology and the Department of Chemistry and Biochemistry, University of Oklahoma, 101 Stephenson Parkway, Norman, Oklahoma, USA 73019*
[b]*Department of Chemistry and Chemical Biology, Stevens Institute of Technology, 1 Castle Point Terrace, Hoboken, New Jersey, USA 07030*
[c]*Department of Chemistry, Brandeis University, 415 South Street, Waltham, Massachusetts, USA 024531*

Insertions of small molecules into metal-carbon bonds ([M]–R; [M] = metal complex, R = alkyl/aryl) to generate derivatives of the form [M]–E–R (E = inserting small molecule) serve as pathways for the generation of new element-carbon bonds [1]. Indeed, such small molecule insertions are well-documented for coordination and non-porphyrin organometallic compounds in both stoichiometric [2] and catalytic reactions [3]. It is somewhat surprising that such small molecule insertions into organometallic *porphyrin*-carbon bonds are not as common, with examples reported for CO/CO_2 [4] and SO_2 [5]. Curiously, no examples had been reported for insertions of NO_x species into metalloporphyrin-carbon bonds prior to our work in this area; reviewed in [6]. Using a "solid crystal + NO gas" methodology, we show that the biological signaling agent nitric oxide (NO) can insert into the metal-carbon bond of a synthetic organometallic porphyrin complex (por)M(aryl) (M = group 9 metal) to generate its nitrosoarene (por)M(ArNO) derivative that was characterized by IR spectroscopy and X-ray crystallography. Density functional theory (DFT) calculations were employed to provide insight into the NO insertion process, and the results suggest that a pre-coordination of NO prior to insertion (i.e., migratory insertion) is not a requirement for the NO insertion to occur. The molecular structure of the identified transition state (TS) reveals details of geometrical changes in the (por)M(Ar) TS that primes it for the NO insertion reaction. The calculated molecular orbitals provide insight into this NO insertion reaction process. Extention of this NO insertion reaction to other organometallic systems will be presented. [Funded by the U.S. National Science Foundation (grants CHE-2154603 and -1900181 to GBRA, and -2102071 to YS) and the U.S. National Institutes of Health (grant GM085774 to YZ)]

REFERENCES

1. Wojcicki, A. Insertion Reactions of Transition Metal-Carbon σ-Bonded Compounds II. *Adv. Organomet. Chem.* **1974**, *12*, 31-81.
2. Rabinovich, D. General Classification of Organometallic Reactions. In *Comprehensive Organometallic Chemistry III*, Mingos, D. M. P., Crabtree, R. H. Eds.; Vol. 1; Elsevier, 2007; pp 93-117.
3. Stanley, G. G. Reaction Mechanisms of Multistep Catalytic Cycles. In *Comprehensive Organometallic Chemistry III*, Mingos, D. M. P., Crabtree, R. H. Eds.; Vol. 1; Elsevier, 2007; pp 119-140.
4. Arafa, I. M.; Shin, K.; Goff, H. M. Carbon Monoxide and Carbon Dioxide Carbon-Metal Bond Insertion Chemistry of Alkyliron(III) Porphyrin Complexes. *J. Am. Chem. Soc.* **1988**, *110*, 5228-5229.
5. Xu, N.; Lilly, J.; Powell, D. R.; Richter-Addo, G. B. Synthesis, Characterization, and Infrared Reflectance Spectroelectrochemistry of Organoruthenium Nitrosyl Porphyrins. *Organometallics* **2012**, *31*, 827-834.
6. Xu, N.; Richter-Addo, G. B. Interactions of Nitrosoalkanes/arenes, Nitrosamines, Nitrosothiols, and Alkyl Nitrites with Metals. *Prog. Inorg. Chem.* **2014**, *59*, 381-445.

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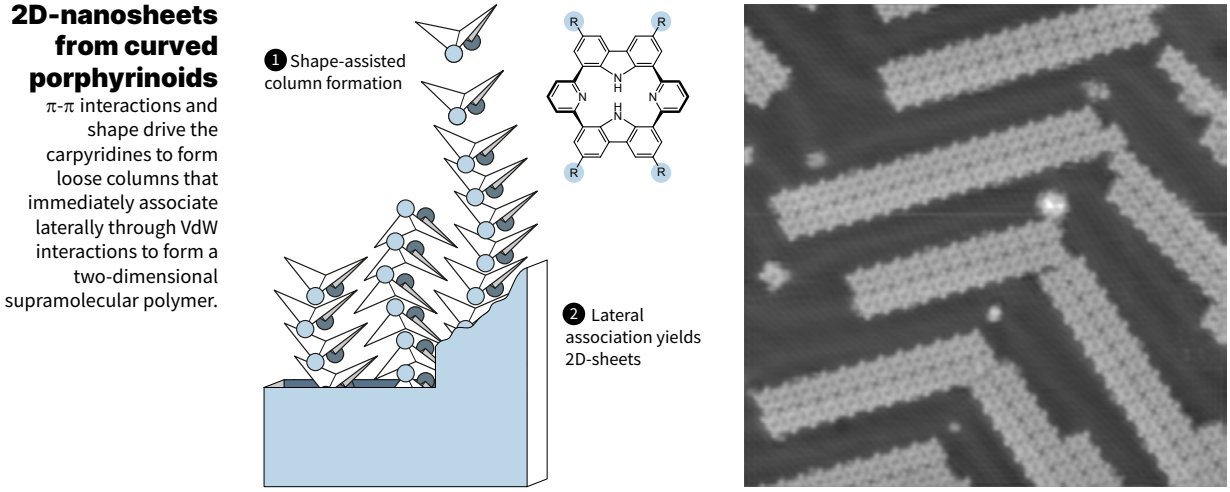
How Bending Porphyrinoids Leads to Extraordinary Order

Michel Rickhaus[a]

[a]*University of Geneva, Department of Organic Chemistry, Geneva, Switzerland*

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In a typical self-assembly setting, a core is decorated by suitable sidechains that induce supramolecular polymerization. While this approach has led to spectacular assemblies, the core has almost always been seen as a rigid platform from which to append functionality rather than as an integral, defining part of the unit. The core mission of our group is to investigate the role that molecular topography – the form– plays in the assembly process. With emphasis on synthetic solutions, we construct π-topographies that we think to be beneficial to supramolecular polymerization.



We were recently[1-3] able to demonstrate that indeed, a simple negatively curved porphyrinoid building block (about 2 nm wide, including sidechains) can instigate order on the micrometer(!) scale with astonishing aspect ratios (about 1:1000:100'000) and edge-definition by simple dropcasting (toluene). The paradigmatic shift is that these soft matter monolayered sheets/flakes are not held together by conventionally employed non-covalent interactions like hydrogen-, ionic, or coordinative-bonding. By using curved π-systems, we succeeded in driving these assemblies to high order mainly by π–π interactions and demonstrated that rational tailoring yields different tertiary structures. I will share key (form)-concepts for π-systems to act as information carriers for shape-assisted self-assembly, insights into our current systems and how these represent the first steps into controlled supramolecular synthesis.

REFERENCES

[1] J. F. Woods/L. Gallego, P. Pfister, M. Maaloum, A. Vargas Jentzsch, M. Rickhaus, *Nature Commun.* **2022**, *13*, 3681

[2] J. F. Woods, L. Gallego, A. Maisch, D. Renggli, C. Cuocci, O. Blacque, G. Steinfeld, A. Kaech, B. B. Spingler, A. Vargas Jentzsch, M. Rickhaus, *Nature Commun.* **2023**, *14*, 4725

[3] L. Gallego, J. F. Woods, R. Butti, P. Szwedziak, A. Vargas Jentzsch, M. Rickhaus *Angew. Chem. Int Ed* **2024,** *63*, e202318879

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Heme-Dependent Iron Mobilization from Bacterioferritin Is Essential for Bacterial Metabolic Homeostasis and Viability

Mario Rivera[a]

[a]*Louisina State University*

Iron metabolism relies on the storage of Fe(III) in bacterioferritin and its regulated mobilization as Fe(II) to meet cellular metabolic demands. In *Pseudomonas aeruginosa*, iron release from bacterioferritin (Bfr) requires binding of a dedicated ferredoxin (Bfd) and heme-mediated electron transfer from Bfd to Fe(III) stored within the interior cavity of bacterioferritin, enabling its reduction and release as soluble Fe(II). We present evidence that deletion of *bfd* causes irreversible sequestration of Fe(III) within Bfr, resulting in intracellular iron starvation, widespread metabolic dysregulation, and defective biofilm development. Consistent with these findings, treatment of mature *P. aeruginosa* biofilms with recently identified small-molecule inhibitors that disrupt the Bfr–Bfd interaction leads to efficient killing of biofilm-embedded cells. Structural and sequence analyses reveal strong conservation of the Bfd binding interface on bacterioferritin from *P. aeruginosa* and *Acinetobacter baumannii*, suggesting that inhibition of this interaction may be broadly effective. In support of this idea, susceptibility testing confirms activity of these inhibitors against *A. baumannii*.

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From innovative molecular photocathodes to photoelectrochemical cell for unassisted CO_2 reduction

Marc Robert[a,b]

[a]*Sorbonne Université, CNRS, Institut Parisien de Chimie Moléculaire (IPCM), 75005 Paris, France*
[a]*Institut Universitaire de France (IUF), 75005 Paris, France*

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Reduction of carbon dioxide has as main objective the production of useful chemicals and fuels - renewable fuels - in which solar energy would be stored. Molecular catalysts can be employed to reach this goal, either in photochemical or electrochemical (or combined) contexts. They may in particular provide excellent selectivity thanks to easy tuning of the electronic properties at the metal and of the ligand second and third coordination sphere. Based on thorough mechanistic studies, we have shown that such molecular catalysts (e.g. metalated porphyrins and phthalocyanines) may be tuned for generating all C1 products, including formaldehyde, methanol and methane, but also C2+ products and more complex molecules, including sugars. [1-6]

In this lecture, our strategy to immobilize molecular catalysts onto innovative photoelectrode will be discussed, as well as our recent results regarding the design of photoelectrochemical cells in which the CO_2 catalytic reduction occurs selectively without applying any external bias. [7-9]

REFERENCES

1. J. Bonin, M. Robert et al. *Nature* **2017**, *548*, 74
2. C. Berlinguette, M. Robert et al. *Science* **2019**, *365*, 367
3. T. F. Jaramillo, M. Robert et al. *Angew. Chem. Int. Ed.* **2019**, *58*, 16172
4. M. Robert et al. *J. Am. Chem. Soc.* **2024**, *146*, 22129
5. M. Robert, M. Abdinejad, T. Burdyny et al., *Nat. Catal.* **2024**, *7*, 1109
6. S. Bontemps, M. Robert et al., *Chem. Sci.* **2025**, *16*, 22996
7. P.B. Pati, E. Boutin, M. Robert et al., *Nat. Commun.* **2020**, 11:3499.
8. H. Ichou, L. Choubrac, F. Odobel, N. Barreau, M. Robert et al., *Angew. Chem. Int. Ed.* **2025**, e202506060
9. M. Robert, N. Barreau, F. Odobel et al., submitted

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Supramolecular Assemblies and Devices based on Subporphyrazines

M. Salomé Rodríguez-Morgade,[a,b] Gema Pérez de Bustos,[a] Julia Arnanz,[c] Tomás Torres,[a,b] Inés Corral,[b,c] Alberto Concellón[d,e]

[a]*Departamento de Química Orgánica, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain*
[b]*Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain*
[c]*Departamento de Química, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain*
[d]*Departamento de Química Orgánica, Universidad de Zaragoza, 50009 Zaragoza, Spain*
[e]*Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, 50009 Zaragoza, Spain*

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Among the different subporphyrinoid classes, subporphyrazines (SubPzs) stand out because of their distinctive structural and chemical features, which make them highly versatile materials. In particular, SubPzs exhibit exceptional electronic tunability through peripheral functionalization, arising from the unusually strong influence of peripheral substituents on the SubPz π-system [1]. Moreover, SubPzs contain a quasi-isolated C_β=C_β bond that is not part of the 14 π-electron circuit, providing an additional handle for the chemical manipulation of these macrocycles [2].
Furthermore, axial functionalization of SubPzs via direct treatment of chloro-SubPzs proceeds efficiently, offering a useful strategy to introduce diverse physical, chemical, and supramolecular properties [3, 4]. Finally, SubPzs display a pronounced tendency to self-assemble into columnar stacks, forming crystalline phases whose nature (solid or liquid) and organization depend on their peripheral and axial substitution patterns [1, 5].
By exploiting all of these features through controlled chemical transformations, we are developing photo-, thermo-, and redox-responsive supramolecular systems and devices that exhibit pronounced and/or reversible modulation of the characteristic SubPz fluorescence, photosensitizing ability, and absorption properties. As a representative example, we are designing and investigating switchable near-infrared absorbers based on SubPz–DTE systems, in which a dithienylethene (DTE) unit reversibly activates the near-infrared absorption of the SubPz core [2, 6]. Recent advances in the use of SubPzs as building blocks for these and other supramolecular applications are presented.

REFERENCES

1. E. Caballero, D. Guzmán, T. Torres, M. S. Rodríguez-Morgade, *J. Org. Chem.* **2020**, *85*, 1948.
2. E. Cañizares-Espada, G. Pérez de Bustos, K. Naoda, A. Osuka, T. Torres, M. S. Rodríguez-Morgade, *Org. Lett.* **2024**, *26*, 955.
3. S. Ben Ahmed, G. Pérez de Bustos, J. Pina, T. Torres, M. S. Rodríguez-Morgade, *ChemPlusChem* **2024**, *89*, e202300779.
4. M. S. Rodríguez-Morgade, C. G. Claessens, A. Medina, D. González-Rodríguez, E. Gutierrez-Puebla, A. Monge, I. Alkorta, J. Elguero and T. Torres, *Chem. Eur. J.* **2008**, *14*, 1342.
5. M. S. Rodríguez-Morgade, S. Esperanza, T. Torres and J. Barberá, *Chem. Eur. J.*, **2005**, *11*, 354.
6. M. Irie, T. Fukaminato, K. Matsuda, S. Kobatake, *Chem. Rev.* **2014**, *114*, 12174.

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Synthesis and Properties of Trinuclear Complexes Based on Iron(II) Octaethyltetrapyrazinoporphyrazine with 3d and 4f Metals

Romanenko N.R.[a], **Faraonov M.A.**[a], **Konarev D.V.**[a]

[a]*Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry, Russian Academy of Sciences (FRC PCPMC RAS), Academician Semenov Ave. 1, 142432 Chernogolovka, Moscow Region, Russian Federation*

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Tetrapyrazinoporphyrazines are macrocyclic molecules containing twelve nitrogen atoms at the periphery of the macrocycle, which can act as coordination sites for various metal ions.

In the present work, iron(II) octaethyltetrapyrazinoporphyrazine ($Fe^{II}Et_8TPyzPz$) was employed for the synthesis of multimetallic paramagnetic homo- and heteronuclear coordination complexes. For the first time, compounds of the compositions $\{TBA^+\}_2[Fe^{II}(I^-)_2(Et_8TPyzPz)^{2-}\cdot(Fe^{II}I_2)_2]^{2-}$ (**1**), $\{TBA^+\}_2[Fe^{II}(I^-)_2(Et_8TPyzPz)^{2-}\cdot(Co^{II}I_2)_2]^{2-}$ (**2**), and $\{TBA^+\}_2[Fe^{II}(Et_8TPyzPz)^{2-}\cdot(Dy^{III}I_3)_2]^{2-}\cdot4C_6H_4Cl_2$ (**3**) were obtained via the reaction of $Et_8TPyzPzFe^{II}$ with Fe^{II}, Co^{II}, and Dy^{III} iodides in the presence of tetrabutylammonium iodide.

The complexes were isolated as single crystals, which enabled investigation of their molecular and crystal structures as well as their magnetic properties.

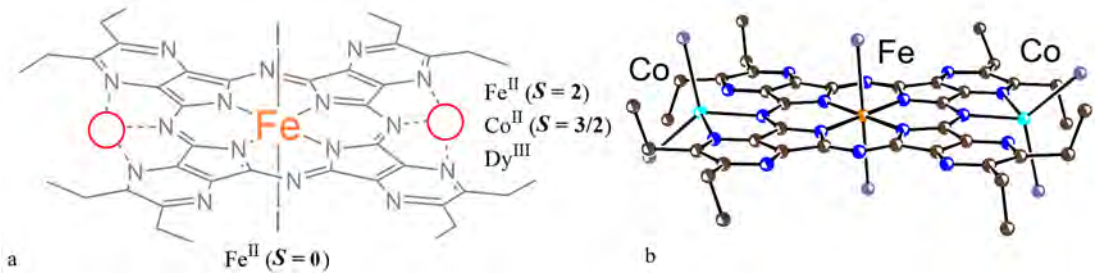


Fig. 1. Schematic representation of the obtained complexes (a); molecular structure of the complex $[Fe^{II}(I^-)_2(Et_8TPyzPz)^{2-}\cdot(Co^{II}I_2)_2]^{2-}$ (b).

It was established that the central iron(II) atom in the $Et_8TPyzPzFe^{2+}$ molecule forms four short N–Fe bonds (1.917–1.927 Å) and two longer I–Fe bonds (2.68 Å) in the complexes. Two molecules of the corresponding metal iodide coordinate to the periphery of the $Et_8TPyzPz$ macrocycle, forming M–N_{meso} and M–$N_{pyrazine}$ bonds (2.14 and 2.42 Å for Fe(II) in **1**; 2.10 and 2.16 Å for Co(II)) in **2** (Fig. 1). In complex 3, the Dy(III) atoms are coordinated simultaneously to three nitrogen atoms, forming M–N bonds with lengths in the range of 2.43–2.75 Å (Fig. 1).

The complexes contain a low-spin diamagnetic central Fe(II) ion and high-spin peripheral Fe(II), Co(II), and Dy(III) centers, which are antiferromagnetically coupled through the diamagnetic $(Et_8TPyzPz)^{2-}$ ligand (Fig. 1a).

This work was supported by the Russian Science Foundation (Grant No. 25-73-10128).

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Optical Properties of Individual Chlorophylls and Phthalocyanines Probed at the Atomic Scale

Anna Roslawska[a]

[a]*Max Planck Institute for Solid State Research, Stuttgart, Germany*

Light-matter interaction is essential for mechanisms such as luminescence, photosynthesis, and energy harvesting, defining the emission characteristics of molecular systems and governing the conversion of energy between photons and electrons. While these processes are intensively studied and employed, little is known about their dependence on atomic-scale properties since reaching such precision in optics is extremely demanding. This challenge is nowadays overcome thanks to the combination of optical spectroscopy with scanning probe microscopy, which profits from the extreme field enhancement provided by the tip, enabling atomic-scale optics. In my talk, I will discuss how this approach can be applied to probe the optical properties of individual phthalocyanine [1-3] and chlorophyll molecules.

REFERENCES

1. A. Rosławska, T. Neuman, B. Doppagne, A. Borisov, M. Romeo, F. Scheurer, J. Aizpurua, G. Schull, Phys. Rev. X, 12, 011012, 2022.
2. K. Kaiser, S. Jiang, M. Romeo, F. Scheurer, G. Schull, A. Rosławska, Phys. Rev. Lett. 133, 156902, 2024.
3. A. Rosławska, K. Kaiser, M. Romeo, E. Devaux, F. Scheurer, S. Berciaud, T. Neuman, G. Schull, Nat. Nanotechnol., 19, 738-743, 2024.

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Redox Gating of Proton Translocation in Cytochrome *c* Oxidase

Denis L. Rousseau, Izumi Ishigami, and Syun-Ru Yeh

Department of Biochemistry, Albert Einstein College of Medicine, Bronx, NY 10461 USA

Proton translocation in cytochrome *c* oxidase is tightly coupled to electron transfer, yet the molecular gate that mediates this coupling has remained elusive. We propose a heme *a* redox-gate mechanism in which rotation of the heme *a* farnesyl side chain provides the structural switch that links electron flow to proton pumping [1]. In the reduced state, the farnesyl hydroxyl group forms a hydrogen bond with S34. Upon oxidation, following electron transfer from heme *a* to the binuclear center, the farnesyl sidechain rotates by ~120° to form a new hydrogen bond with S382, concomitant with proton release to a proton-loading site. Reduction of heme *a* reverses this rotation, driving proton uptake from the N-side of the membrane via the H-channel and resetting the system. Each electron transferred through heme *a* therefore drives one cycle of proton loading and release, ensuring tight coupling and preventing proton backflow. This mechanism establishes heme *a* and its redox-driven farnesyl rotation as a central structural element in proton translocation.

REFERENCES

1. Rousseau, D.L., I. Ishigami, and S.-R. Yeh, *Structural and functional mechanisms of cytochrome c oxidase. J Inorg Biochem*, 2025. **262**: p. 112730.

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Enzyme under siege: Mechanistic insights into the inhibition of vitamin B_{12}-dependent methylmalonyl CoA mutase

Markus Ruetz[a], **Ruma Banerjee**[a]

[a]*Department of Biological Chemistry, University of Michigan, Ann Arbor, MI, USA*

Vitamin B_{12} (cobalamin) is an essential cofactor for two human enzymes: cytosolic methionine synthase and mitochondrial methylmalonyl-CoA mutase (MMUT). MMUT catalyzes the conversion of methylmalonyl-CoA to succinyl-CoA via a remarkable adenosylcobalamin (AdoCbl)-dependent radical mechanism, initiated by the homolytic cleavage of the cobalt – carbon bond to yield a highly reactive 5′-deoxyadenosyl radical.

We reveal how two distinct coenzyme A derivatives — itaconyl-CoA and malyl-CoA — inhibit MMUT activity through unique mechanisms. Itaconyl-CoA, the thioester of the immunomodulatory metabolite itaconate, acts as a mechanism-based suicide inhibitor by forming a covalent adduct with the 5′-deoxyadenosyl radical. Remarkably, this radical addition product is stable in air, enabling crystallographic visualization of the elusive 5′-deoxyadenosyl radical for the first time.[1]

We also explore malyl-CoA, a thioester derivative of the tricarboxylic acid cycle intermediate malate, as a novel MMUT inhibitor.[2] While initial spectroscopic analysis revealed similarities to itaconyl-CoA, the absence of a reactive carbon–carbon double bond in malyl-CoA pointed to a distinct mechanism of enzyme inactivation. Our integrated structural and biophysical analyses reveal an unprecedented redox-based inactivation pathway for MMUT. Importantly, whereas inhibition by itaconyl-CoA is irreversible, MMUT inactivation by malyl-CoA can be reversed by the enzyme's intrinsic repair system.

These insights provide new aspects of B_{12}-dependent enzymology and demonstrate the intricate control MMUT exerts over its native radical intermediates

REFERENCES

1. M. Ruetz *et al*., *Science* **366**, 589 (2019)
2. C.M. Griffith *et al.*, *Nat. Chem. Biol*. **21**, 906 (2025)

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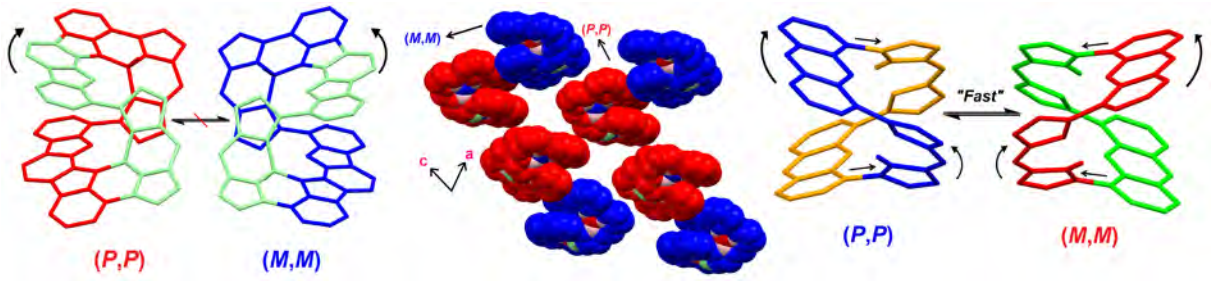
Persistent *vs.* Induced Helical Chirality in *bis*-Subporphyrin-like Boron(III) Complexes and Anthracene linked Twisted Macrocycles

Gokulnath Sabapathi[a]

School of Chemistry, IISER Thiruvananthapuram, Maruthamala PO, Vithura, Kerala-695 551, INDIA
E-mail: gokul@iisertvm.ac.in

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Enantiopure helical systems have potential applications in circularly polarized luminescent materials (CPL), nonlinear optical materials, spin filters, circularly polarized organic light emitting diodes (CP-OLEDs), and bio-imaging applications. Chirality in porphyrinoid is an emerging field recently realized with large and flexible macrocycles with appropriate linking subunits.[1] The optical resolution of these macrocycles is often difficult to achieve owing to their dynamic interconversion between two conformers.[2] In the first part of my talk, the synthesis, structure, and chiroptical properties of a conformationally stable, helically locked, and twisted Cyclo[2]Dipyrrins **1** containing two dipyrrin units separated by anthracene subunits. Macrocycle **1** is a non-planar, crystallizes as a racemic mixture and adopts a highly twisted non-planar conformation. High racemization energy barrier enabled facile optical resolution. The (*P*,*P*) and (*M*,*M*) enantiomers show moderate chiroptical properties, such as absorption dissymmetry factors in the order of 10^{-3} and luminescence dissymmetry factors of 3.8 x 10^{-3} and 2.9 x 10^{-3} at 702 nm respectively.[3] Subsequently, an interesting '*figure-eight*' conformation of another anthracene embedded macrocycle and its bis-BF_2 complex were obtained. Enantiopure forms were obtained due to its low racemization energy barriers. Therefore, the freebase were treated with chiral acids and obtained the CD response corresponding to the induced chirality of these acid bound structures. Next, I will introduce a new '*figure-eight*' helically chiral macrocycle embedded with two dihydroindolo(2,3-a)carbazole subunits. The unprecedented rigidification was achieved through $\mathbf{BF_2}$ complexation and subsequent fusion led to **2·BF**. The rigid chiral framework of **2·BF** complex allowed chiral separation of enantiomers *P*,*P* and *M*,*M* which displayed chiral response in the near-IR region with Δε of up to 150 M^{-1} cm^{-1} at 692 nm.[4]



REFERENCES

[1] S. E. Penty, M. A. Zwijnenburg, G. R. F. Orton, P. Stachelek, R. Pal, Y. Xie, S. L. Griffin, T. A. Barendt, *J. Am. Chem. Soc.* **2022**, *144*, 12290-12298. [2] Y. Li, A. Yagi, K. Itami, *J. Am. Chem. Soc.* **2020,** *142*, 3246-3253. [3] Anjana P. Nambiar, P. Nag, R. Mariam Ipe, S. Reddy Vennapusa, S. Gokulnath, *Angew. Chem. Int. Ed.* **2023**, 10.1002/anie.202306566 [4] Aswini Spergen, P. V. Bal, A. K. Shameer Shameem, A. Joshy, A. P. Nambiar, A. P. Andrews, S. Gokulnath, *Chem. Sci.* **2025**, *16*, 19164-19171

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Water Soluble Phosphorus(V) Phthalocyanines: From Synthesis to Biomedical Applications

Safonova E.A.[a], Polovkova M.A.[a], Ovchenkova A.E.[a,b], Gorshkov E.V.[a,b,c], Akasov R.A.[d], Tsivadze A.Yu. [a,c], Gorbunova Yu.G.[a,b,c]

[a] *Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Moscow, Russia*
[b] *Lomonosov Moscow State University, Moscow, Russia*
[c] *Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow, Russia*
[d] *Department of Biochemistry, Petrovsky Medical University, Moscow, Russia*

ORALS

The development of efficient photosensitizers for biophotonics is an important task for contemporary science at the interface of chemistry, biology, and medicine. Phthalocyanines (Pcs) are well-known photosensitizers, including drugs that have already been used in clinical practice. The introduction of a P(V) atom leads to a significant bathochromic shift of the absorbance maximum of Pcs as well as an increase in their solubility due to the appearance of a positive charge and axial ligands. Nevertheless, no examples of water-soluble phosphorus(V) phthalocyanines (PcPs) had been published prior to our work.

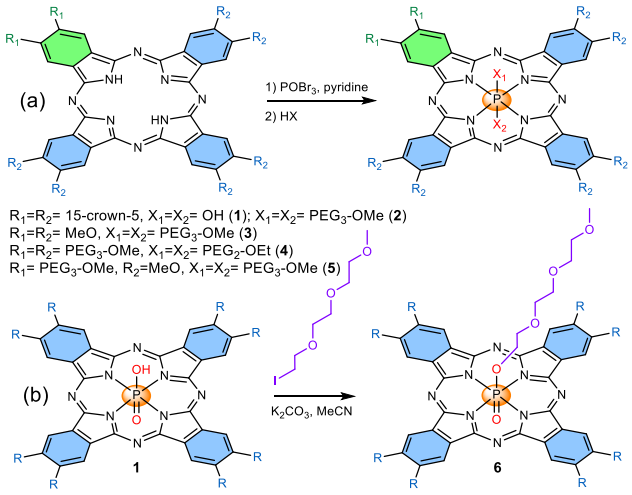


Fig. 1. Syntesis of watersoluble P(V) phthalocyanines.

Here we present different approaches to the synthesis of water-soluble PcPs and the investigation of their photophysical, photochemical, and cytotoxic properties. The first way to improve the water solubility is the introduction of hydrophilic substituents (crown-ethers, polyethylene-glycol ethers) in peripheral positions of the Pc ring or as axial ligands on P(V) atom (Fig 1a). Besides that, the ability to substitute OH-axial ligands via alkylation was demonstrated for the first time on the example of complex **1** (Fig 1b), which opens up wide possibilities for further modification, including the introduction of specific targeting groups for different biomedical applications. All obtained compounds possess solubility in water, absorbance, and fluorescence in the red and near-IR range of the spectrum.

Biological studies demonstrated that complex **3** possesses a photocytotoxic effect on tumor cells, with an IC_{50} of 3 μM (MCF-7). On the other hand, complex **2** is a non-toxic, efficient photoinitiator of biocompatible polymers, photocrosslinking [1]. Therefore, obtained PcPs are promising photosensitizers for PDT and photoinitiators for tissue engineering.

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REFERENCES

1. Safonova *et al*., Dyes and Pigments, **2024**, 225, 112095

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Photocatalytic CO_2 Reduction in Aqueous Media

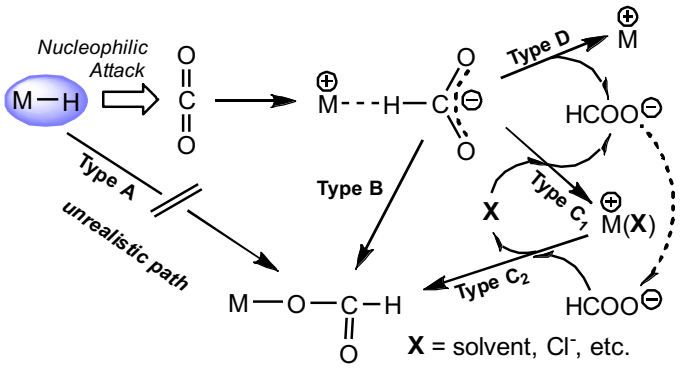
Ken Sakai

Department of Chemistry, Faculty of Science, Kyushu University, Fukuoka, Japan.
Email: ksakai@chem.kyushu-univ.jp

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We previously demonstrated that a water-soluble heteroleptic copper(I) photosensitizer is highly effective in photocatalytic CO_2 reduction into CO in the presence of a water soluble cobalt porphyrin catalyst even in fully aqueous media. Our study demonstrated high selectivity in CO_2 reduction versus water reduction (Sel_{CO2}=90%) with a high turnover number (TON_{CO}=4000, 12 h). Ionic interaction of the photosensitizer in aqueous media was also utilized to enhance the photocatalytic efficiency [1-6].

Our recent interest has concentrated on the selective formate formation due to its potential application in reversible hydrogen storage technology. However, selective catalysts for CO_2-to-HCOOH conversion is quite limited due to the predominant formation of CO_2^{2-}-coordinated intermediates. Although the formate formation was classically supposed to take place via the insertion of CO_2 into a metal-hydride bond (Type A), this concept is rather misleading since formate often forms via the nucleophilic attack of a metal-hydride (M-H) at the carbon center of CO_2 (Types B-D). Indeed, our recent studies strongly suggest that CO_2 reduction to formate undergoes via the M-H attack with the lack of any O(formate)-coordinated products and directly ends up with the release of formate (Type D) [7,8]. The most remarkable finding in our report lies in the drastic change in the product selectivity induced by switching the reaction media from non-aqueous to aqueous/organic phase, leading to demonstrate outstanding efficiencies of $[Rh^{III}Cp^*(dihydroxy\text{-}bpy)Cl]^+$ in CO_2-to-HCOOH conversion [8]. This sytem, tother with the Ni-NHC catalyst [7], became good examples of demonstrating the fact that the nucleophilic attack of metal hydride to the carbon center of CO_2 is a key to have a high formate selectivity versus the CO or H_2 production in CO_2 reduction .



REFERENCES

1. A. Call, M. Cibian, K. Yamamoto, T. Nakazono, K. Yamauchi, K. Sakai, ***ACS Catal.*** **2019**, *9*, 4867-4874.
2. X. Zhang, M. Cibian, A. Call, K. Yamauchi, K. Sakai, ***ACS Catal.*** **2019**, *9*, 11263-11273.
3. X. Zhang, K. Yamauchi, K. Sakai, ***ACS Catal.*** **2021**, *11*, 10436-10449.
4. A. Call, M. Cibian, K. Yamauchi, K. Sakai, ***Sustainable Energy Fuels*** **2022**, *6*, 2160-2164.
5. F. Sueyoshi, X. Zhang, K. Yamauchi, K. Sakai, ***Angew. Chem. Int. Ed.*** **2023**, *62*, e202217807.
6. J.-W. Wang, X. Zhang, L. Velasco, M. Karnahl, Z. Li, Z.-M. Luo, Y. Huang, J. Yu, W. Hu, X. Zhang, K. Yamauchi, K. Sakai, D. Moonshiram, G. Ouyang, ***J. Am. Chem. Soc. Au*** **2023**, *3*, 1984-1997.
7. C. Liao, K. Yamauchi, K. Sakai, ***ACS Catal.*** **2024**, *14*, 11131-11137.
8. D. Lee, K. Yamauchi, K. Sakai, ***J. Am. Chem. Soc.*** **2024**, *146*, 31597-31611.

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Synthesis of C_{3+} products via the electrochemical CO_2 reduction using dinuclear Cu(I) molecular catalysts

Naonari Sakamoto[a], Keita Sekizawa[a], Soichi Shirai[a], Takamasa Nonaka[a], Takeo Arai[a], Shunsuke Sato[a], Takeshi Morikawa[a]

[a] *Toyota Central R&D Labs., Inc., Japan*

The CO_2 reduction reaction (CO_2RR) is regarded as a promising approach to address climate change and energy depletion by converting greenhouse gases into valuable chemicals and fuels. Compared to the well-established systems for two-electron reduction products such as carbon monoxide and formic acid [1-2], reports on molecular catalysts capable of producing multi-electron C_2 products (e.g., ethylene and ethanol) through C–C bond formation remain limited. Most existing studies have focused on rigidly structured catalysts such as coordination polymers [3–4]. Moreover, molecular catalysts that do facilitate C_2 product formation often undergo decomposition during the reaction, converting into metallic species. Therefore, to achieve efficient C_2 product formation using molecular catalysts, it is critical to develop new catalysts that maintain structural integrity under operating conditions.

In this study, we report a bromide-bridged dinuclear copper molecular catalyst exhibiting high structural stability for CO_2/CO reduction, capable of producing C_{3+} products such as propanol [5]. Operando X-ray absorption fine structure (XAFS) and other spectroscopic analyses reveal that the catalyst maintains a stable Cu(I) state during the reaction, preventing degradation. Furthermore, operando spectroscopy based on localized surface plasmon resonance identifies key C_2 and C_3 coupling intermediates essential for C_3 product formation. These findings are supported by experiments using $^{13}CO_2$-labeled operando analysis. Density functional theory (DFT) calculations suggest a mechanism in which C_3 species are formed at room temperature through C–C coupling at the dinuclear Cu center. The proposed mechanism indicates that the CO_2/CO-reduced intermediate bridges the two copper centers, dynamically adjusting the Cu–Cu distance during the reaction. Propanol is formed via C–C coupling at this bridging site within the flexible dinuclear structure. Our discovery of a robust molecular catalyst capable of forming C_{3+} products provides valuable design insights for next-generation catalysts targeting multi-carbon CO_2RR pathways.

REFERENCES

1. T. Nishi, N. Sakamoto, K. Sekizawa, T. Morikawa, S. Sato, *ChemSusChem* **2025**, 18, e202401082.
2. J. Jung, K. W. Lee, N. Sakamoto, S. Kaliyamoorthy, T. Wakabayashi, K. Kamada, K. Sekizawa, S. Sato, T. M Suzuki, T. Morikawa, S. Saito, *EES Catal*, **2025**, 3, 254-258.
3. N. Sakamoto, Y. F. Nishimura, T. Nonaka, M. Ohashi, N. Ishida, K. Kitazumi, Y. Kato, K. Sekizawa, T. Morikawa, T. Arai, *ACS Catal.*, **2020**, 10(18), 10412-10419.
4. N. Sakamoto, K. Sekizawa, S. Sato, M. Ohashi, T. Nonaka, Y. F Nishimura, K. Kitazumi, T. Morikawa, T. Arai, *J. Catal.*, **2021**, 404, 12-17.
5. N. Sakamoto, K. Sekizawa, S. Shirai, T. Nonaka, T. Arai, S. Sato, T. Morikawa, *Nat. Catal.,* **2024**, 7, 574-584.

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Towards Near-Infrared Luminescence via Charge-Transfer Design in Complexes

Eri Sakuda [a]

[a] *Division of Chemistry and Materials Science, Graduate School of Integrated Science and Technology, Nagasaki University*

ORALS

The design of luminescent transition-metal complexes with well-defined excited-state properties has long been an important topic in coordination and photophysical chemistry. In particular, controlling charge-transfer (CT) excited states is essential for accessing long-wavelength and near-infrared (NIR) emission, yet this remains a challenging task due to the complex interplay between metal centers, ligand frameworks, and molecular geometry.

Over the past several years, we have been engaged in the synthesis and photophysical investigation of a variety of dipyrrin-based transition-metal complexes, with the aim of clarifying how ligand design and coordination environment influence their electronic and excited-state properties. Dipyrrin ligands provide a versatile platform because of their strong visible absorption and structural flexibility, allowing systematic modification through both metal selection and ligand functionalization. Among the transition metals explored, platinum(II) offers a particularly interesting case owing to its rich coordination chemistry and potential involvement in charge-transfer excited states.

In this talk, I will focus on our recent studies on dipyrrin-based platinum(II) complexes that exhibit near-infrared emission associated with charge-transfer excited states. By introducing electron-accepting arylborane units into a dipyrrin ligand framework, we obtained homoleptic platinum(II) complexes showing enhanced absorption in the visible region and characteristic emission behavior. Although these complexes share the same molecular composition, they were found to adopt different coordination geometries.

Interestingly, these subtle structural differences lead to pronounced changes in photophysical properties. One form exhibits weak and structured red emission, whereas another displays broad NIR emission extending to longer wavelengths. Spectroscopic experiments combined with theoretical analyses suggest that the NIR emission originates from a low-energy triplet excited state with appreciable charge-transfer character involving both the platinum center and the boron-containing substituents. This observation indicates that coordination geometry, in addition to ligand electronics, can play an important role in determining the nature of the emissive excited state.

The talk concludes with a brief review of recent and ongoing efforts to explore related dipyrrin-based compounds. While still in their early stages, these studies may contribute to a deeper understanding.

REFERENCES

1. K. Takaki, E. Sakuda, A. Ito, S. Horiuchi, Y. Arikawa, K. Umakoshi, *Inorg. Chem.,* **2019**, *58(21)*, 14542-14550.
2. K. Takaki, E. Sakuda, A. Ito, S. Horiuchi, Y. Arikawa, K. Umakoshi, *RSC Advances*, **2021**, *11(11)*, 6259-6267.
3. K. Takaki, E. Sakuda, A. Ito, S. Horiuchi, Y. Arikawa, K. Umakoshi, *Chem. Lett. 49(8)*, 905-908.

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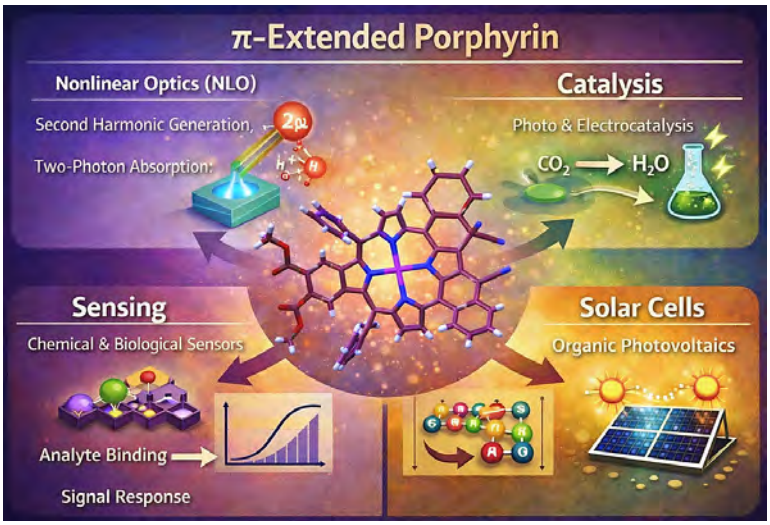
Synthesis of π-Extended Porphyrins and Their Applications in Catalysis, Nonlinear Optics, Solar Cells and Sensing

Muniappan Sankar

Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 24667, India

ORALS

π-Extended porphyrins represent a rapidly expanding class of functional macrocycles distinguished by their tunable electronic structures, rich redox chemistry and extraordinary photophysical responses.[1] Strategic π-extension achieved through *β*- and *meso*-fusion, annulation, and installation of electron-rich/withdrawing substituents modulates molecular planarity, frontier orbital energetics, and charge-transfer characteristics, yielding exceptional optoelectronic properties, enhanced near-infrared absorption, tunable redox behaviour and significant nonlinear optical responses. These attributes directly enable diverse, high-performance applications. They serve as superior electrocatalysts for ORR and CO_2 conversion.[1d,1e] Their intense, environment-sensitive luminescence and redox activity make them excellent platforms for chemical and biological sensing. Furthermore, their high hyperpolarizabilities and charge-transfer character are exploited in NLO devices for optical limiting and switching. Advances in synthetic methodologies, mechanistic understanding and device integration continue to broaden the technological relevance of π-extended porphyrins. Their engineered architecture and multifunctionality underscore their potential as a unifying molecular platform for next-generation optoelectronic, catalytic and sensing technologies.[1f,1g]



REFERENCES

1. (a) A. S. Bulbul *et al*. *Chem. Eur. J*., **2025**, *31*, e202403473. (b) M. Sankar *et al*. *Inorg. Chem.,* **2024**, *63*, 17967−17982. (c) D. Pinjari *et al*. *Angew. Chem. Int. Ed.*, 2020, **59**, 23697−23705. (d) D. K. Singh *et al*. *ACS Catal.*, 2023, *13,* 4155−4167. (e) A. S. Bulbul *et al*. *Chem. Commun.*, **2024**, *60*, 3146-3149. (f) M. Sankar *et al*. *Inorg. Chem.,* **2025**, *64*, 25216-25227. (g) M. Sankar *et al*. *Inorg. Chem.,* **2026**, *65*, 1812-1823.

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Weak magnetic coupling interactions and spin dynamics in photochromic porphyrin-based quantum logic gates

Fabio Santanni[a], Christian Teutloff[b], Kseniia Mamaeva[c], Anja C. Gotzen[a], Brendan Twamley[a], A. Louise Bradley[c], Robert Bittl[b], Mathias O. Senge[a]

[a]*School of Chemistry, Trinity Biomedical Sciences Institute, Trinity College Dublin, D02R590 Dublin, Ireland.*
[b]*Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany.*
[c]*School of Physics and AMBER, SFI Research Center, Trinity College Dublin, D02PN40, Dublin, Ireland*

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In the last few decades, molecular magnets have attracted attention as potential electron-spin-based quantum bits (qubits) due to their tunable quantum properties and the possibility of realizing multi-qubit systems via chemistry. For instance, meso-meso-linked metalloporphyrin dimers have been proven to fulfil the optimal requirements for the realization of two-qubit quantum logic gates [1]. However, it is crucial to obtain qubit-qubit couplings that can be triggered on demand to provide scalable, adaptable quantum solutions, thereby avoiding potential drawbacks of permanently coupled systems, e.g., uncontrollable many-body dynamics. Recently, triplet states have been proposed as an efficient means to trigger exchange interactions in hybrid VO-F-VO (VO = vanadyl, F = free-base) meso-meso-linked porphyrin trimers [2]. Nevertheless, additional synthetic efforts are required to achieve a fully controllable architecture in which the effects of photogenerated states can be turned off on demand.
Alternatively, the electrocyclization reactivity of photochromic diarylethene units can be exploited to switch magnetic interactions between molecular qubits while maintaining a weak-coupling regime [3]. We present here a novel approach based on metalloporphyrin (M = Cu, VO) and radical (R) units bridged by a photocromic diarylethene core (PC) as potential photoswitchable multi-qubit systems. Magnetic interactions can be modulated upon irradiation with UV or visible light, i.e., upon cyclization or cycloreversion of the photochromic core (Figure 1). A complete characterization and rationalization of the optical and magnetic behavior of M-PC-M and Cu-PC-R systems through a multitechnique approach based on optical spectroscopy, transient absorption, electron paramagnetic resonance, and DFT calculations is reported. Our results show that magnetic interactions in M-PC-M and M-PC-R systems can be tuned via photocyclization, with the smallest detectable variation of the interaction down to ≈ 20 MHz.

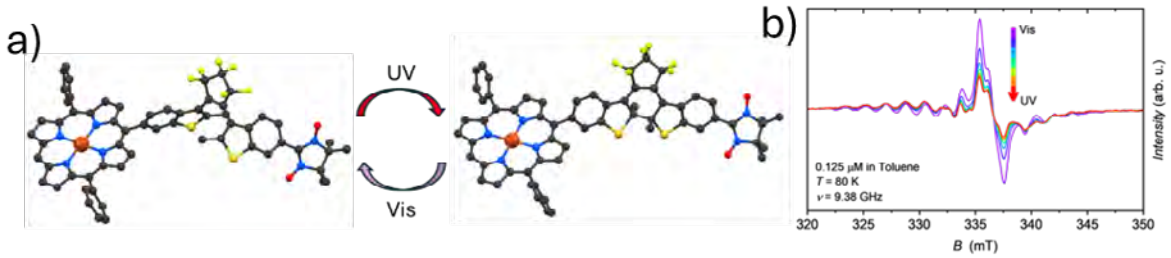


Figure 1. a) Optimized structures of Cu-PC-R in the open and closed forms. b) Variation of the CW-EPR spectrum of the Cu-PC-R system on the left upon photocyclization at 365 nm.

REFERENCES

1. F. Santanni, A. Privitera, *Adv. Optical Mater.* **2024**, 12, 2303036
2. A. Privitera, A. Chiesa, F. Santanni, *et al. J. Am. Chem. Soc.* **2025**, in press
3. J. Salinas Uber, *et al. Chem. Eur. J.* **2017**, 23, 13648 – 13659

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Extending Photoinduced Magnetism to Light Lanthanide through Porphyrin Excited States

Anas Santria[a,b], **Tsuyoshi Ashida**[a], **Naoto Ishikawa**[a]

[a]*Department of Chemistry, Graduate School of Science, The University of Osaka*
[b]*Reseach Center for Molecular Chemistry, National Research and Innovation Agency*

Lanthanide single-molecule magnetism is generally understood as a ground-state phenomenon governed by strong spin-orbit coupling and crystal-field anisotropy, primarily associated with heavy rare earth ions [1-2]. Previous studies have revealed that magnetically active states can also emerge upon photoexcitation, through an interaction between the angular momentum of the localized 4f electronic system (**J**) and the orbital angular momentum generated in the π-π* excited states of porphyrin and phthalocyanine ligands (**L**) [3-5]. This photoinduced **J**-**L** interaction represents a fundamentally different class of magnetic coupling, activated only under irradiation and inaccessible to conventional static magnetometry.

In this contribution, we extend the concept of excited-state magnetism to porphyrin complexes of lighter lanthanide ions, including Nd(III), Pr(III), and Sm(III), which differ in the ground state magnetic properties from the heavier lanthanide ions more commonly studied in single-molecule magnetism. Variable-temperature, variable-magnetic-field magnetic circular dichroism (VTVH-MCD) measurements reveal clear signatures of magnetically active excited states in the porphyrin π-π* transitions, demonstrating that orbital angular momentum generated upon photoexcitation can effectively couple even to moderately anisotropic 4f systems.

These results demonstrate that photoinduced **J**-**L** coupling is not limited to heavy lanthanides and can also be observed in porphyrin complexes of lighter rare-earth ions. This extension broadens the experimentally accessible scope of excited-state magnetism and provides a useful platform for systematically examining how differences in 4f electronic structure influence magneto-optical responses in photoexcited lanthanide-porphyrin complexes.

REFERENCES

1. N. Ishikawa, M. Sugita, T. Ishikawa, S-Y. Koshiwara, Y. Kaizu, *J. Am. Chem. Soc.* 2003, 125, 29, 8694–8695.
2. C.A.P. Goodwin, F. Ortu, D. Reta, N.F. Chilton, D.P. Mills, *Nature,* 2017, 548, 439−442.
3. K. Kizaki, H. Ozawa, T. Kobayashi, R. Matsuoka, Y. Sakaguchi, A. Fuyuhiro, T. Fukuda, N. Ishikawa, *Chem. Commun.* 2017, 53, 6168−6171.
4. A. Santria, N. Ishikawa, *Inorg. Chem*. 2020, 59, 14326–14336.
5. A. Santria, N. Ishikawa, *Inorg. Chem*. 2021, 60, 14418–14425.

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Cancer Immunity Activation in Photodynamic Therapy Using Talaporfin Sodium

Makiko Sasaki[a], **Mamoru Tanaka**[a], **Hiromi Kataoka**[a]

[a]*Department of Gastroenterology and Metabolism, Nagoya City University Graduate School of Medical Sciences, Nagoya, Japan.*

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[Introduction] Photodynamic therapy (PDT) has been reported to enhance antitumor innate immune responses [1]; however, the underlying mechanisms remain incompletely understood. [Objective] We performed a basic analysis of the antitumor effects of PDT using talaporfin sodium (TS) as an inducer of immunogenic cell death, and investigated the synergistic effects of TS-PDT in combination with an immune checkpoint inhibitor, an anti–programmed cell death 1 (anti–PD-1) antibody. [Methods] TS-PDT was performed using gastrointestinal cancer cell lines, HCT116, KYSE30, and MC38. The induction of damage-associated molecular patterns, including calreticulin, high-mobility group box 1, heat shock proteins, and ATP, was evaluated using fluorescence immunostaining, flow cytometry, and ELISA. The synergistic antitumor effects of TS-PDT combined with an anti–PD-1 antibody were assessed using live-cell imaging. Tumor growth suppression by combination therapy was compared with that of TS-PDT or anti–PD-1 antibody monotherapy using a syngeneic mouse model. [Results] TS-PDT induced several damage-associated molecular patterns *in vitro*. In addition, TS-PDT upregulated PD-L1 expression on tumor cells *in vivo* and exhibited efficient synergistic antitumor effects when combined with an anti–PD-1 antibody. [Conclusion] The combination of TS-PDT and an anti–PD-1 antibody has the potential to activate cytotoxic T lymphocytes and suppress tumor growth more effectively than either monotherapy. In this presentation, we aim to provide an overview of PDT as a cancer immunotherapy and to introduce clinical cases of combination treatment with TS-PDT and anti–PD-1 antibody.

REFERENCES

1. Mamoru Tanaka, Hiromi Kataoka, Shigenobu Yano et al. Immunogenic cell death due to a new photodynamic therapy (PDT) with glycoconjugated chlorin (G-chlorin). Oncotarget. 2016 Jul 26;7(30):47242-47251.

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Phthalocyanine-Based Molecular Materials: From Symmetry Breaking to Hole Transporting Agents

Ángela Sastre-Santos,[a] Lydia Ferrer,[a] Adrián Hernandez, [a] Desiré Molina,[a] Javier Ortiz,[a] José Garcés-Garcés,[a] Jorge Follana-Berná,[a] Fernando Fernández-Lázaro [a]

[a]Área de Química Orgánica, Instituto de Bioingeniería, Universidad Miguel Hernández, Elche 03202 (Alicante), Spain. E-mail: asastre@umh.es

Recent scientific efforts have highlighted intriguing physical phenomena that can be leveraged to enhance the performance of organic photovoltaic devices. Among these, photoinduced symmetry-breaking charge transfer (SBCT) has emerged as a particularly promising mechanism. Phthalocyanines, owing to their remarkable structural and chemical tunability, can also exhibit SBCT. Despite this potential, only a limited number of examples have been reported in the literature, underscoring the need for further investigation. [1].

Recently, significant progress has been achieved in the fabrication of highly efficient perovskite solar cells, while major challenges, such as the commercial viability of exotic materials and their instability, remain as obstacles. Hole-transporting materials (HTMs) pose a tricky choice for the fabrication of efficient solar cells, and the cost-ineffective Spiro-OMeTAD remains the most obvious candidate. Semiconductor molecules, such as metallophthalocyanines (MPcs) [2], appeared as a promising class of p-type material, since they are less expensive and more stable.

In this communication, we will present the synthesis of novel MPcs dimers with different geometries and bridges to explore SBCT occurrence (Fig. 1a) [3], and also MPcs systems as efficient, stable, and low-cost HTMs in PSCs (Fig. 1b).[4]

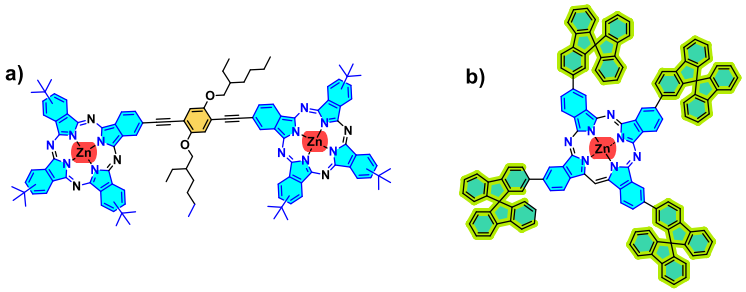


Figure 1. Example of synthesized ZnPcs for (a) symmetry-breaking charge transfer studies and (b) as HTM in PSC.

REFERENCES

1. M. Cacioppo, T. Scharl, L. Đorđević, A. Cadranel, F. Arcudi, D. M. Guldi, M. Prato, *Angew Chem Int Ed* **2020**, *59*, 12779–12784.
2. D. Molina, J. Follana, Á. Sastre-Santos, *J. Mater. Chem. C*, **2023**, *10*, 11975–11982.
3. R. R. Kaswan, D. Molina, L. Ferrer-López, J. Ortiz, P. A. Karr, Á. Sastre-Santos, F. D'Souza, *Ange. Chem. Int. Ed.,* **2025**. e202502516.
4. a) M. Gassara, L. Ferrer, L. Lezama, D. Molina, J. Ortiz, S.Kazim, Á. Sastre-Santos, S. Ahmad, *Solar RRL*, **2025**, 9:e2500418. b) M. Gassara, J. Garcés-Garcés, L. Lezama, J. Ortiz, F. Fernández-Lázaro, S.Kazim, Á. Sastre-Santos, S. Ahmad, *J. Mater. Chem. C* **2025**, *13*, 1704-1712. c) A. Hernández, J. G. Sánchez, J. Ortiz, E. Martínez-Ferrero, E. Palomares, Á. Sastre-Santos, J. Mater. Chem.C **2025**, *13*, 15977-15987.

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Directly Linked 2,2′-Bipyridine–Porphyrin Architectures: Molecular Platforms for Multinuclear Assembly

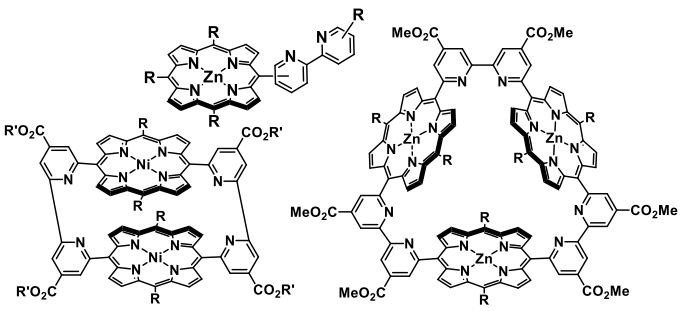
Akiharu Satake[a] and Leonardo Hayato Foianesi-Takeshige[a]

[a]*Department of Chemistry, Faculty of Science Division II, Tokyo University of Science*

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Linking 2,2′-bipyridine (bpy) directly to porphyrins offers a compact molecular platform for constructing heteromultinuclear complexes relevant to multi-electron catalysis. While polymeric bpy–porphyrin materials have recently emerged as robust catalysts, directly linked molecular systems allow precise, position-specific structure–function analysis. Here we present the synthesis and properties of 4-, 5-, and 6-linked bpy–porphyrin architectures spanning meso-linked bisporphyrins and cyclic oligomers, including a 6-linked zinc porphyrin cyclic trimer and a 6-linked nickel porphyrin cyclic dimer. Direct C–C linkage enforces close spatial proximity without extended π-conjugation, producing rigid scaffolds in which the bpy and metalloporphyrin coordination sites co-localize on one face, enhancing cooperativity while constraining coordination volume.

We demonstrate position-dependent coordination chemistry ($Ru(bpy)_3$-type complexation [1][2]; steric exclusion of $PdCl_2$ [3]), selective mono-metalation of Re(I) carbonyls due to a retarded second insertion (enabling chromatographic isolation) [4], and distinctive retention hierarchies on functionalized silica [5]. Hydrolysis of pendant esters to carboxylic acids yields hydrogen-bonded organic frameworks (HOFs), motivating expansion to MOF-like porous assemblies. For CO_2 reduction, directly linked porphyrin–phenanthroline and bpy systems show high activity [6][7]; increasing electron density on the bpy fragment (via ester reduction) accelerates catalysis [4]. Notably, zinc porphyrin derivatives exhibit room-temperature phosphorescence[6]; comparative studies across 4-, 5-, and 6-linked isomers identify the 5-linked variant as the most active[7], and ongoing work examines possible correlations between phosphorescence dynamics and catalytic performance[8][9]. These results establish directly linked bpy–porphyrin molecules and their higher-order assemblies as tunable, robust platforms for multi-electron transformations.



REFERENCES

1. Kitagishi, H.; Satake, A.; Kobuke, Y. *Inorg. Chem.* **2004**, *43* (11), 3394–3405.
2. Fukuda, S.; Satake, A.; Kobuke, Y. *Thin Solid Films*, **2006**, 499, 263–268.
3. Tomohiro, Y.; Satake, A.; Kobuke, Y. *J. Org. Chem.* **2001**, *66* (25), 8442–8446.
4. Kuramochi, Y.; Tanahashi, K.; Satake, A. *Chem. Eur. J.* **2024**, *30* (10), DOI: 10.1002/chem.202303324.
5. Satake, A.; Seino, K.; Odaka, Y.; Katagami, Y.; Kuramochi, Y. *Bull. Chem. Soc. Jpn.* **2023**, *96* (2), 156–167.
6. Kuramochi, Y.; Fujisawa, Y.; Satake, A. *J. Am. Chem. Soc.* **2020**, *142* (2), 705–709.
7. Kuramochi, Y. et al. *Chem. Sci.* **2023**, *14* (33), 8743–8765.
8. Honda, T. et al. *Inorg. Chem.* **2024**, *63* (50), 23524–23533.
9. Kuramochi, Y.; Satake, A. *Catalysts* **2023**, *13* (2), DOI: 10.3390/catal13020282.

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The development of a soft X-ray microscope for imaging of heme iron in living cells to understand its dynamics

Hitomi Sawai[a, b]

[a] *Department of Chemistry, Graduate School of Science, Osaka Metropolitan University*
[b] *Institute for Molecular Science, National Institutes of Natural Sciences*

Heme (an iron-bound tetrapyrrole) is essential for regulating cellular functions and bioenergetics. There are various heme-containing proteins, which perform a variety of essential catalytic and noncatalytic functions in almost all organisms. Well-known functions of heme proteins include electron transfer, respiration, and oxygen transport, and heme enzymes are central to many metabolic pathways in biology. In addition, new roles of heme were discovered in the transcriptional regulation of the circadian clock, control of the immune response, neurodegeneration and aging, gas sensing, and gating ion channels. Given the wide-ranging control heme exerts over many cellular processes, it follows that its supply and distribution within the cell must be highly coordinated to respond to demand and ensure the timely availability of the tetrapyrrole. One remaining question is how the distribution and concentrations of hemes are regulated in living cells. To address this point, we have developed a novel technique to quantitatively visualize the localization and distribution of heme iron in living cells without destruction.

Methods such as fluorescent probes, Raman microscopy, and mass spectrometry imaging are being developed to visualize biomolecules in living cells. However, these methods have certain drawbacks, including low sensitivity and cell destruction during measurement using powerful lasers. Additionally, these methods cannot analyze the electronic state of elements. Currently, there is no method that can simultaneously analyze the distribution and quantity of elements in living cells, as well as their chemical bonds and redox state. To overcome these issues, we developed a new technique that uses soft X-ray imaging to visualize metal compounds, including heme iron, in living cells by chemical species. Soft X-rays, characterized by their low energy (200–2,000 eV) and wavelengths (0.6–10 nm), minimize radiation damage in living cells compared to hard X-rays. Their energy range aligns with the absorption edges of essential elements, making them ideal for in-cell metal imaging. A new "contact-type soft X-ray microscope" has been developed at the UVSOR synchrotron facility to visualize elements in living cells. In this microscope, living cells are directly placed on a Ce:YAG scintillator, converting transmitted X-ray images into visible-light images captured by a CMOS camera. By changing the photon energies, the energy dependence of transmitted images can be obtained, and a three-dimensional XANES mapping can be extracted for each pixel of the image.

In this talk, I will introduce a novel imaging method for metal species in living cells by presenting results from mapping the distribution and local concentrations of heme iron in a single red blood cell isolated from bovine and gallus blood.

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On-Surface Synthesis: Extrinsic Catalysis and Molecular Conformation

Alex Saywell

School of Physics & Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom

On-surface synthesis (OSS) provides alternative reaction pathways to those available in solution-phase chemistry and enables the fabrication of extended molecular architectures with unique electronic and magnetic properties [1-3]. Conventional OSS relies on metallic substrates acting as both catalyst and support; however, strong molecule–substrate hybridisation often suppresses the desired molecular functionality. Here, we explore an approach to decouple catalytic activity from substrate electronic structure by patterning a non-metallic surface (highly oriented pyrolytic graphite (HOPG)) with gold nanoclusters.

Building on our recent work investiogating the reaction progress of halogenated prohyrins on coinage metals [4,5], we employ brominated tetraphenyl porphyrin (BrxTPP) as a model reaction precursor, and investigate Ullmann-type coupling reactions initiated by an extrinsic Au catalyst. Our methodology combines temperature-programmed X-ray photoelectron spectroscopy (TP-XPS) and near-edge X-ray absorption fine structure (NEXAFS) to monitor key mechanistic steps, including debromination and metalation. We discuss C–Br bond dissociation on Au-HOPG, alongside porphyrin metalation (formation of Au-TPP), and highlight distinct temperature-dependent behavior differing from that observed on Au(111) [4]. This study provides insight into the role of spatially localised catalysts in OSS and offers a route to fabricating covalently bonded nanostructures on non-metallic substrates, preserving optoelectronic properties by minimising molecule–substrate hybridisation.

In addition, we present a complementary study utilising normal incidence X-ray standing wave (NIXSW) analysis to probe chemically specific structural changes during Ullmann-type reactions of halogenated porphyrins on metallic substrates. In previous work we combined the chemical sensitivity of XPS with the structural characterisation provided by NIXSW to probe key atomic species during an on-surface reaction [6]. Here, we examine conformational changes within BrxTPP during dehalogenation and metalation, focusing on N, C, and Br atoms within the molecules at different reaction stages. This approach offers mechanistic insight into the molecule–surface interactions and conformational changes that underpin on-surface synthesis.

Together, these studies combine mechanistic insight into multi-step on-surface reactions with an approach to spatially localised catalysis, offering a pathway to fabricate covalently bonded nanostructures on non-metallic substrates while preserving optoelectronic properties.

REFERENCES

1. Chen, Z.; Narita, A.; Müllen, K. *Adv. Mater.* **2020**, 32, 2001893.
2. Grill, L.; Hecht, S. *Nature Chemistry* **2020**, *12*, 115–130.
3. Sweetman, A.; Champness, N. R.; Saywell, A. *Chem. Soc. Rev.* **2020**, *49*, 4189–4202.
4. Frampton, E. S. et al. *ACS Appl. Nano Mater.* **2025**, 8 (24), 12608.
5. Frampton, E. S. et al *J. Phys. Chem. Lett.* **2025**, 16 5012–5017.
6. Judd, C. J. et al. *Commun Chem* **2020**, 3, 166.

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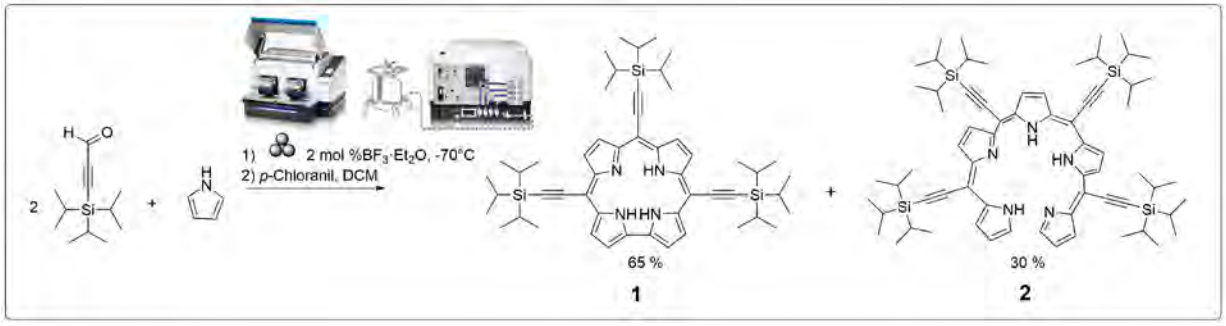


Cryogenic Mechanochemistry for Sustainable Porphyrinoid Catalyst Design in Energy Storage Systems

Wolfgang Schöfberger[a], Sankit Vala, Simon Offenthaler, Adrian Dorniak[a]

[a] *Johannes Kepler University Linz, Institute of Organic Chemistry, Altenberger Straße 69, 4040, Linz, Austria.*

Tetrapyrrolic macrocycles such as porphyrins, corroles, and phthalocyanines are foundational to molecular catalysis, optoelectronics, and energy conversion. Yet their synthesis remains constrained by the extensive use of solvents and poor scalability.
This talk introduces a cryogenic mechanochemical approach—an energy-efficient, solvent-free strategy that leverages low-temperature ball milling to promote selective macrocyclization (Scheme 1).



Scheme 1. Cryo-mechanochemical synthesis of free-base 5, 10, 15 - tris(3-(triisopropylsilyl)ethynyl)corrole.

We show that cryogenic conditions stabilize transient intermediates, enhancing yields and enabling access to otherwise inaccessible meso-substituted derivatives. Using a temperature-controlled milling platform (Retsch MM 500 control with cryoPad), we systematically explore the influence of temperature and mechanical parameters on porphyrinoid formation.[1] The resulting metallated macrocycles will be integrated into 1D–3D conductive networks and evaluated as electrocatalysts. By merging cryogenic control with mechanochemistry, this work pioneers a sustainable synthetic route toward complex macrocycles and their functional catalytic architectures.[2] The approach aligns with global and national (Austria 2040) energy transition goals, advancing low-emission pathways for next-generation energy storage and conversion technologies.

REFERENCES

1. Cryo-mechanochemical synthesis of free-base and metal A_3-corroles and A_4-porphyrins: A solvent-free approach, A. Dorniak and W. Schöfberger, Journal of Porphyrins and Phthalocyanines, 2025. https://doi.org/10.1142/S1088424625500208
2. Tuning ORR selectivity of π-Conjugated Cobalt Corroles from $2e^-$ to $4e^-$, H. Sun, H. Awada, H. Lei, A. Aljabour, L. Song, S. Offenthaler, R. Cao, and W. Schöfberger, Materials Today Catalysis 2024, 4, 100038. https://doi.org/10.1016/j.mtcata.2023.100038

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Iron insertion in bacterial ferrochelatases: Active site architecture and iron-sulfur cluster

Federico Sebastiani[a,b], Alice Cassiani[c], Andrea Dali[a], Thomas Gabler[c], Maurizio Becucci[a,b], Paul G. Furtműller[c], Stefan Hofbauer[c], Giulietta Smulevich[a]

[a]*Department of Chemistry "U. Schiff", University of Florence, Via della Lastruccia 3, Sesto Fiorentino (FI), Italy*
[b]*The European Laboratory for Non-Linear Spectroscopy (LENS), Via N. Carrara 1, Sesto Fiorentino (FI), Italy*
[c]*Department of Natural Sciences and Sustainable Resources, BOKU University, Muthgasse 18, Wien, Austria*

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During infections, heme biosynthesis is a highly efficient strategy for bacterial pathogens to survive, since heme is otherwise sequestered by high-affinity host proteins [1]. Monoderm bacteria, namely Firmicutes and Actinobacteria, utilize the coproporphyrin-dependent (CPD) pathway for heme biosynthesis, while eukaryotes predominantly use the long-known protoporphyrin-dependent (PPD) pathway [2]. In both pathways, the incorporation of ferrous iron into tetrapyrrole macrocycles is catalysed by homologous enzymes, namely protoporphyrin- and coproporphyrin-ferrochelatases (PpfCs and CpfCs), which have different physiological substrates. While PpfC, as the last enzyme of the PPD pathway, converts protoporphyrin IX into iron protoporphyrin IX (heme *b*), CpfC inserts Fe^{2+} ions into coproporphyrin III, yielding ferric coproporphyrin III [3], which is eventually decarboxylated by the coproheme decarboxylase enzyme to obtain heme *b* [4].
Despite strong structural similarities between fCs from different bacterial clades, a recent study on the distribution of [2Fe-2S] cluster motif in ferrochelatases genomic sequences highlighted that, for Gram-positive bacteria, the cluster is completely missing in firmicute CpfCs and it is only present in a fraction of actinobacterial CpfCs, which display the same cysteine motif in the C-terminal extension as human PpfC [5]. Human PpfC is a homodimer protein containing in each subunit a [2Fe-2S] cluster coordinated by one cysteine in the internal core of the protein and three cysteines in the external C-terminal region [6], whose removal results in a loss of activity [7] and clinical consequences [8]. However, the function of prokaryotic clusters remains elusive, and, to our knowledge, it was only experimentally investigated before the discovery of the CPD pathway.
Here, we present an in-depth study of the active site of the actinobacterial CpfC from *C. diphtheriae*, which possesses a [2Fe-2S] cluster, using UV-vis and resonance Raman spectroscopies. Variants lacking the cluster have also been investigated to elucidate its effects on porphyrin binding, active-site stability, and enzyme activity. Further, an X-ray crystallographic structure of apo-*Cd*CpfC is presented and compared with structural and spectroscopic data on wild-type and selected distal variants from firmicute *L. monocytogenes* in the apo- and substrate-bound forms [9,10] to elucidate the role of conserved residues for iron insertion and stabilization of the heme cavity.

REFERENCES

1. J.E. Choby, E.P. Skaar – *J. Mol. Biol.* (2016) 428, 3408.
2. H.A. Dailey, S. Gerdes, T.A. Dailey et al. – *Proc. Natl. Acad. Sci. USA* (2015) 112, 2210.
3. T. Gabler, A. Dali, F. Sebastiani et al. - *Protein Science* (2023) 32, e4788.
4. F. Sebastiani, H. Michlits, B. Lier et al. – *Biophys. J.* (2021) 120, 3600.
5. R.S. Weerth, A.E. Medlock, H.A. Dailey – *J. Biol. Chem.* (2021) 297, 101017.
6. B.R. Crouse, V.M. Sellers, M.G. Finnegan et al. – *Biochemistry* (1996) 35, 16222.
7. H.A. Dailey, V.M. Sellers, T.A. Dailey - *J. Biol. Chem.* (1994) 269, 390.
8. X. Schneider-Yin, L. Gouya, M. Dorsey, U. Rüfenacht, J-C. Deybach, G.C. Ferreira – *Blood* (2000) 96, 1545.
9. T. Gabler, F. Sebastiani, J. Helm et al. - *FEBS J.* (2022) 289, 1680.
10. A. Dali, T. Gabler, F. Sebastiani et al. - *Protein Science* (2024) 32, e4534.

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Photochemical approaches for strengthening cancer immunotherapy

Pål K. Selbo[1]

[1]*Department of Radiation Biology, Institute for Cancer Research, The Norwegian Radium Hospital, Oslo University Hospital, Oslo, Norway*

Photodynamic therapy (PDT) combines photosensitizers with light activation to generate reactive oxygen species (ROS), producing targeted cytotoxicity. Beyond direct tumour destruction and vascular shutdown, PDT enhances cancer immunotherapy by inducing immunogenic cell death, local inflammation, and immune cell recruitment into light-exposed tumour tissue [1]. I will demonstrate how PDT significantly improves Bacille Calmette-Guérin (BCG) efficacy in bladder cancer treatment. In a preclinical bladder cancer model, combining BCG with PDT markedly increased antitumour activity. In vitro and in vivo studies using MB49 carcinoma cells and immunocompetent mice show that BCG–photosensitizer complexes elicit dose-dependent cytotoxicity, drive transcriptomic reprogramming, and achieve durable tumour remission in some animals. Photochemical internalisation (PCI), an advanced endosomal escape technology derived from PDT, further expands therapeutic potential. PCI uses photosensitisers that accumulate in endolysosomal membranes and, upon light activation, generate ROS that rupture these compartments, releasing entrapped agents into the cytosol [2]. This enables efficient endosomal escape of peptide antigens, driving robust activation of antigen-specific CD8+ T cells and supporting effective anti-cancer vaccine strategies. In preclinical models, fimaporfin-based PCI combined with tumour-specific peptides and adjuvants induces strong, durable anti-tumour immune responses [3-4]. I will also highlight proof-of-concept work on PCI-mediated, light-controlled elimination of PD-L1-expressing suppressor cells, offering a selective strategy to improve specificity and overcome resistance in PD-L1-positive cancers [5]. Together, PDT and PCI underscore the versatility and translational promise of photochemical strategies. Integrating light-based modalities with immunotherapy opens new opportunities to enhance tumour-specific immune responses and achieve improved clinical outcomes across diverse cancer types.

REFERENCES

1. Selbo PK, Korbelik M. Enhancing antitumour immunity with photodynamic therapy. Photochem Photobiol Sci. 2025 Feb;24(2):227-234. doi: 10.1007/s43630-025-00690-2.
2. Selbo PK, Weyergang A, Høgset A, Norum OJ, Berstad MB, Vikdal M, Berg K. Photochemical internalization provides time- and space-controlled endolysosomal escape of therapeutic molecules. J Control Release. 2010 Nov 20;148(1):2-12. doi: 10.1016/j.jconrel.2010.06.008.
3. Håkerud M, Selbo PK, Waeckerle-Men Y, Contassot E, Dziunycz P, Kündig TM, Høgset A, Johansen P. Photosensitisation facilitates cross-priming of adjuvant-free protein vaccines and stimulation of tumour-suppressing CD8 T cells. J Control Release. 2015 Jan 28;198:10-7. doi: 10.1016/j.jconrel.2014.11.032.
4. Haug M, Brede G, Håkerud M, Nedberg AG, Gederaas OA, Flo TH, Edwards VT, Selbo PK, Høgset A, Halaas Ø. Photochemical Internalization of Peptide Antigens Provides a Novel Strategy to Realize Therapeutic Cancer Vaccination. Front Immunol. 2018 Apr 4;9:650. doi: 10.3389/fimmu.2018.00650.
5. Wong JJW, Selbo PK. Light-controlled elimination of PD-L1+ cells. J Photochem Photobiol B. 2021 Dec;225:112355. doi: 10.1016/j.jphotobiol.2021.112355.

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The Isostere Concept in Porphyrin Chemistry

Mathias O. Senge[a,b]

[a]*School of Chemistry, Trinity Biomedical Sciences Instiute, 152-160 Pearse Street, Trinity College Dublin, The University of Dublin, Dublin 2, Ireland*
[b]*Institute for Advanced Study, Technical University Munich, Lichtenbergstraße 2a, 85748 Garching, Germany*

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Classic isosteres are atoms or molecular units with similar shapes and same number of atoms and valence electrons. In modern times the focus of isosterism research has shifted to nonclassical isosteres, i.e., functionally different chemical groups which can be substituted for one another to yield compounds with similar activity [1]. Widely used in medicinal chemistry, typical examples of such 'bioisosteres' are cubane or bicyclo[1.1.1]pentane (BCP) as drop-in replacements of benzene rings. This 'escape from flatland' often gives rise to different binding properties and interaction profiles [2]. Except for synthetic methodological studies [3] this concept has not been explicitly used for the development of novel functional organic materials.

We propose to use the isostere concept as a means to categorize the chemical space of porphyrinoids in combination with Vogel's annulene concept [4].

To aid in the development of this approach we have developed syntheses for porphyrins appended with rigid hydrocarbon (RHC) scaffold molecules [5], porphyrin dyads and donor-acceptor systems bridged by isolating RHC units for electron transfer studies, applications in spintronics, and novel calix-BCP porphyrinoids [6]. Further studies involve the logical spatial construction of 1D, 2D, 3D arrays of organic electronic components using on-surface synthesis [7] and using porphyrinoids as photoactive components together with rigid hydrocarbon linker groups either in solution [6,8], the solid state [9], or interfaces [7,10,11].

REFERENCES

1. G. M. Locke, S. S. R. Bernhard, M. O. Senge, *Chem. Eur. J.* **2019**, *25*, 4590.
2. K. J. Flanagan, S. S. R. Bernhard, S. Plunkett, M. O. Senge, *Chem. Eur. J.* **2019**, 25, 6941; N. Grover, K. J. Flanagan, C. Trujillo, C. J. Kingsbury, M. O. Senge, *Eur. J. Org. Chem.* **2021**, 1113.
3. N. Grover, M. O. Senge, *Synthesis* **2020**, *52*, 3295.
4. E. Vogel, *Pure Appl. Chem.* **1993**, *65*, 143.
5. S. S. R. Bernhard, G. M. Locke, S. Plunkett, A. Meindl, K. J. Flanagan, M. O. Senge, *Chem. Eur. J.* **2018**, *24*, 1026.
6. N. Grover, M. Cheveau, B. Twamley, C. J. Kingsbury, C. M. Mattern, M. O. Senge, *Angew. Chem. Int. Ed.* **2023**, *62*, e202302771.
7. B. Yang, K. Niu, N. Cao, N. Grover, W. Zhao, A. Riss, J. Björk, W. Auwärter, J. V. Barth, M. O. Senge, *Angew. Chem. Int. Ed.* **2023**, *62*, e202218211.
8. N. Grover, G. M. Locke, K. J. Flanagan, M. H. R. Beh, A. Thompson, M. O. Senge, *Chem. Eur. J.* **2020**, *26*, 2405.
9. C. J. Kingsbury, M. O. Senge, *Coord. Chem. Rev.* **2021**, *431*, 213760.
10. M. Ottolini, Z. Anfar, N. Grover, G. Magna, M. Stefanelli, R. Paolesse, M. O. Senge, S. Bettini, L. Valli, R. Oda, G. Giancane, *Nanoscale* **2024**, *16*, 16593.

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Contrasting CO_2 Activation at Low- and High-Valent Metal Centers

Junhyeok Seo

Gwangju Institute of Science and Technology (GIST)

Reducing CO_2 is a key change in both biological and synthetic catalytic systems. When examining the CO_2 reactivity of low-valent Co and Fe centers supported by imino–bipyridyl ligands, carboxylate intermediates tend to form first. This aligns with CO_2 activation pathways often seen in typical transition-metal complexes. Our recent findings show that ligand design is crucial for tuning the proton-coupled electron transfer (PCET) pathways required for CO_2 activation, thereby influencing the overall reaction mechanism. Conversely, when highly Lewis acidic catalytic sites based on high-valent metal ions are used, the formation of carboxylate intermediates becomes less likely. Dithiolene ligands effectively stabilize high-valent metal centers, and CO_2 reactions with dithiolene-supported tungsten complexes mainly produce formate. This reactivity resembles that of the active site in formate dehydrogenases.

In this presentation, we will discuss how different PCET pathways in low-valent systems impact CO_2 activation and highlight the newly discovered selective formation of formate in high-valent metal systems.

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Proton-coupled aromaticity switching

Jonathan L. Sessler[a]

[a]*The University of Texas at Austin*

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Considerable interested is focused on porphyrin analogues that can exist in several different electronic states. In collaboration with several groups, whose contributions are gratefully acknowledged, an emphasis has been made to develop pyrrolic macrocycles that can be switched between formal aromatic, non-aromatic, antiaromatic, and open shell and forms via so-called proton-coupled electron transfer reactions. Early efforts along these lines involved the study of rosarins, but have lately been extended to include other hexapyrrolic macrocycles, various fused, and cage-type systems. Lately, an effort has been made to explore how changes in electronic states can be used to switch on potentially useful biomedical properties, including those associated with photoacoustic imaging.

Collaborations with a number of groups, including those of Profs. Dongho Kim, Juwon Kim, Jong Sung Kim, Shunichi Fukuzumi, T.K. Chandrashekar, Dirk Guldi, Changhee Lee, Jan Jeppesen, Steffen Bähring, Jingqin Chen, Zhao-Xi Wang, Aaron Tondreau, Chuanhu Lei, Hongyu Wang, Jun-long Zhang, Christophe Bucher, Graeme Henkelman, and Tomas Torres, are gratefully acknowledged. Special thanks also go to current and former coworkers, including Yu-Dong Yang, Duong Nguyen, Leah Biwot, Masatoshi Ishida, Calvin Chau, Han-Yuan Gong, Jonathan F. Arambula, Gregory Thiabaud, Sajal Sen, Qing He, Zhan Zhang, Xian-sheng Ke, Xiaofan Ji, Xiaodong Chi, Atanu Jana, Adam Sedgwick, James Brewster, Jungsu Park, and Daniel Mangel. Support for this work is being provided by the National Science Foundation and the Robert A. Welch Foundation.

REFERENCES

1. Ishida, M.; Kim, S.-J.; Preihs, C.; Ohkubo, K.; Lim, J. M.; Lee, B. S.; Park, J. S.; Lynch, V. M.; Roznyatovskiy, V. V.; Sarma, T.; Panda, P.K.; Lee, C. H.; Fukuzumi, S.; Kim, D.; Sessler, J. L. *Nature Chem.* **2013**, *5*, 15. **DOI:** 10.1038/NCHEM.1501
2. Cha, W.-Y.; Kim, T.; Ghosh, A.; Zhang, Z.; Ke, X.-S.; Ali, R.; Lynch, V. M.; Jung, J.; Kim, W.; Lee, S.; Fukuzumi, S.; Park, J. S.; Sessler, J. L.; Chandrashekar, T. K.; Kim, D. "Bicyclic Baird-type Aromaticity," *Nature Chem.* **2017**, *9*, 1243-1248. **DOI**: 10.1038/NCHEM.2834
3. Ke, X.-S.; Kim, T.; He, Q.; Lynch, V. M. Kim, D.; Sessler, J. L. *J. Am. Chem. Soc.* **2018**, *140*, 16455. **DOI:** 10.1021/jacs.8b11158
4. Chen, J.; Sedgwick, A. C.; Sen, S.; Ren, Y.; Sun, Q.; Chau, C.; Arambula, J. F.; Sarma, T.; Song, L.; Sessler, J. L.; Liu, C. *Chem. Sci.* **2021**, *12*, 9916. **DOI**: 10.1039/D1SC01591E
5. Chen, J.; Chen, R.; Chau, C. V.; Sedgwick, A. C.; Xue, Q.; Chen, T.; Zeng, S.; Chen, N.; Wong, K. K. Y.; Song, L.; Ren, Y.; Yang, J.; Sessler, J. L.; Liu, C. *J. Am. Chem. Soc*. **2024**, *146*, 7, 4620. **DOI**: 10.1021/jacs.3c11666
6. Yang, Y.-D.; Zhang, Q.; Chau, C. V.; Yang, J.; Wang, Y.-Y.; Bucher, C.; Henkelman, G. A.; Gong, H.-Y.; Sessler, J. L. "Chemically Mediated Artificial Electron Transport Chain," *ACS Central Science* **2024**, *10*, 1148-1155. **DOI**: 10.1021/acscentsci.4c00165

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Structure of O_2-inactivated Radical B_{12} Diol Dehydratase and Identification of Adenosylcobalamin Degradation Products

Naoki Shibata

Department of Life Science, Graduate School of Science, University of Hyogo

Radical B_{12} enzymes initiate catalysis by activating the cobalt–carbon (Co–C) bond of adenosylcobalamin (AdoCbl), inducing its homolytic cleavage to generate an adenosyl radical, which abstracts a hydrogen atom from the substrate. The holoenzyme of diol dehydratase (DD) is rapidly inactivated by molecular oxygen (O_2) in the absence of substrate [1,2]. Previously, we determined the structure of the DD–AdoCbl complex under anaerobic conditions and obtained structures in which the Co–C bond was cleaved irrespective of the presence or absence of substrate [3]. Diffraction data collection and structural analysis using the crystals prepared under anaerobic conditions indicated, based on the shape of the electron density, that the adenosyl moiety of AdoCbl had been converted to 5′-deoxyadenosine [3].

In the present study, we performed structural analysis using crystals prepared under aerobic conditions. As a result, an unidentified electron density was observed near the 5′-carbon atom (C5′) of the adenosyl moiety under aerobic conditions. Since such electron density was not observed under anaerobic conditions, we hypothesized that O_2-involving reactions led to the addition of an atom or functional group to C5′. To identify products derived from the adenosyl moiety, HPLC analysis was performed. As a result, adenine, adenosine 5′-aldehyde, adenosine, 5′,8-cyclic adenosine, and 5′-deoxyadenosine were detected in crystals prepared under aerobic conditions, with estimated proportions of 2–4%, 44–62%, 2–11%, 4–6%, and 28–37%, respectively. In contrast, crystals obtained under anaerobic conditions contained adenine, 5′,8-cyclic adenosine, and 5′-deoxyadenosine, with estimated proportions of 1–5%, 19–33%, and 66–76%, respectively.

In the case of O_2-inactivation of photo-activated free AdoCbl in solution, adenine, adenosine 5′-aldehyde, adenosine, and 5′-peroxyadenosine have been identified, whereas neither 5′-deoxyadenosine nor 5′,8-cyclic adenosine was detected [2]. Although 5′-deoxyadenosine is one of the enzymatic reaction intermediates, it remains at the catalytic site when the radical is quenched by side reactions, preventing regeneration of AdoCbl [3, 4]. The reason why 5′-peroxyadenosine was not detected in crystals prepared under aerobic conditions remains unclear. However, the detection of 5′-deoxyadenosine may be explained by a reaction of the adenosyl radical with residual substrate, 1,2-propanediol, present in the purified enzyme, resulting in its irreversible formation through mechanism-based inactivation.

REFERENCES

1. P. A. Schwartz, P. A. Frey, *Biochemistry*, **46**, 7293–7301 (2007)
2. T. Toraya, *Chem. Rev*., **103**, 2095-2127 (2003); *Arch. Biochem. Biophys*., **544**, 40–57 (2014)
3. N. Shibata, Y. Sueyoshi, Y. Higuchi, T. Toraya, *Angew. Chem. Int. Ed. Engl*., **57**, 7830–7835 (2018)
4. T. Toraya, N. Tamura, T. Watanabe, M. Yamanishi, N. Hieda, K. Mori, *J. Biochem*., **144**, 437–446 (2008)

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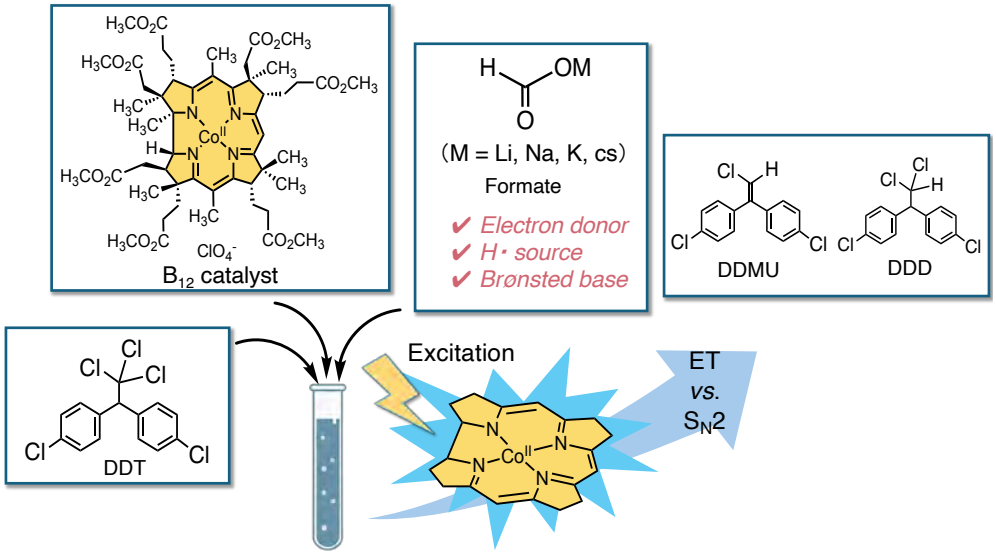
Boosting Photocatalytic DDT Dechlorination by B_{12} Complex with Formate

Hisashi Shimakoshi

Department of Applied Chemistry, Graduate School of Engineering, Kyushu University, Fukuoka, Japan

ORALS

The light-driven alkenylation of trichlorinated organic compounds using a B_{12} catalyst and a formate salt was reported. The formate salt acts as a sacrificial electron donor, hydrogen radical source, and Brønsted base. Trichlorinated organic compounds such as l,l,l-trichloro-2,2-bis(*p*-chlorophenyl)ethane (DDT) were selectively converted into the corresponding monochlorinated alkene, DDMU, under aerobic conditions and at ambient pressure. A mechanistic study revealed that DDT is dechlorinated by B_{12} catalysis to form the mono-dechlorinated product, 1,1-bis(4-chlorophenyl)-2,2-dichloroethane (DDD). Dehydrochlorination of DDD by the formate then forms the final mono-chlorinated alkene, l-chloro-2,2-bis(4-chlorophenyl)ethene (DDMU). An isotope-labeling experiment showed that the hydrogen atom of the formate is incorporated into the final alkene products. To gain an understanding of dechlorination by the B_{12} catalyst, we performed DFT calculations for the reaction of trichlorinated organic compounds with the Co(I) state of B_{12}. The calculations suggest that the electron transfer (ET)-type reaction is energetically favored over the S_N2-type reaction in the dechlorination of trichlorinated organic compounds.



REFERENCES

1. H. Shimakoshi, *Chem. Rec.* **2021**, *21*, 2080.
2. M. Moniruzzaman, H. Shimakoshi *et al*, *Bull. Chem. Soc. Jpn.*, **2021**, *94*, 2784.
3. K. Shichijo, H. Shimakoshi *et al*, *Bull. Chem. Soc. Jpn.*, **2022**, *95*, 1016.
4. H. Shimakoshi *et al*, *Dalton Trans.*, **2004**, 278.
5. H. Shimakoshi *et al*, *Chem. Commun.*, **2011**, *47*, 10921.

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Far-Red and SWIR aza-BODIPY Oligomers and Their Photothermal Properties

Soji Shimizu

Department of Applied Chemistry, Graduate School of Engineering and Center for Molecular Systems (CMS), Kyushu University, Fukuoka 819-0395, Japan (ssoji@cstf.kyushu-u.ac.jp)

Far-red and short-wave infrared (SWIR) chromophores have garnered increasing attention, especially in the fields of bioimaging and phototherapy, due to the high penetration depths of far-red and SWIR lights into biological tissue, small autofluorescence, and low scattering, which enable diagnosis and therapeutics in deep tissue. Owing to the intense absorption and fluorescence in the far-red region, aza-borondipyrromethene (aza-BODIPY) has been found as a structural basis for targeting optical properties in such wavelength regions. Therefore, the synthesis of aza-BODIPY and its analogues has been intensively investigated.[1–3] As a new synthetic method of aza-BODIPY, we have developed a Schiff base-forming reaction of lactam and aza-arylamine.[4] Due to the wide substrate scope, we have developed a variety of novel aza-BODIPY analogues, achieving redshifts of absorption and fluorescence of up to 800 nm and 860 nm, respectively.[5] In this study, to shift the optical properties to longer wavelength regions, we have developed two aza-BODIPY oligomers, **NPAB** and **PP2AB** (Fig. 1). **NPAB** was synthesized from N-Pechmann dye based on our aza-BODIPY synthetic protocol. In contrast, a new stepwise synthetic method was developed to synthesize **PP2AB**. Both compounds exhibited absorption over 860 nm, and the main absorbance of **PP2AB** extended to the SWIR region. Due to the thermal decay of **NPAB** enhanced by the cross-conjugated structure, **NPAB** nanoparticles fabricated with biodegradable PEG-PLGA polymers exhibited a photothermal conversion efficiency of 47%, high photostability, and photoacoustic signals. The cell viability test of the nanoparticles revealed 93% ablation of A549 cancer cells upon NIR laser irradiation.

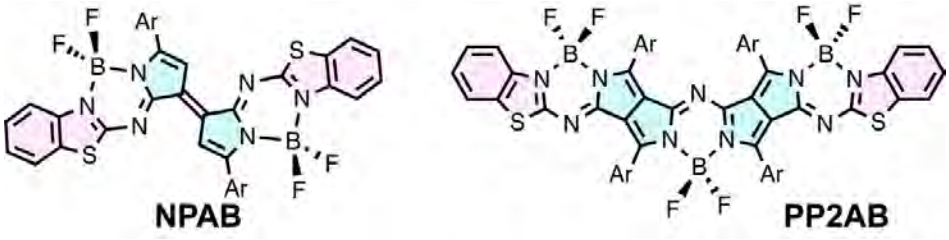


Fig. 1. Structures of **NPAB** and **PP2AB**.

REFERENCES

1. Killoran J, Allen L, Gallagher JF, Gallagher WM, O'Shea DF, *Chem. Commun*. 2002; 1862.
2. Zhao W, Carreira EM, *Angew. Chem., Int. Ed*. 2005; 44: 1677.
3. Donyagina VF, Shimizu S, Kobayashi N, Lukyanets EA, *Tetrahedron Lett*. 2008; 49: 6152.
4. (a) Shimizu S, Iino T, Araki Y, Kobayashi N, *Chem. Commun.* 2013; 49: 1621. (b) Shimizu S, *Chem. Commun*. 2019; 55: 8722.
5. Wang S, Mori S, Nakanotani H, Adachi C, Shimizu S, *Org. Lett*. 2023; 25: 3040.

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An exploration study of practical secondary organic batteries with porphyrinoid electrodes

Ji-Young Shin

Graduate School of Engineering, Nagoya University

ORALS

Porphyrinoid derivatives as active electrode materials have been used to develop an electrochemical understanding relevant to the manufacture of superior secondary organic batteries and to investigate the influence of various electron-conjugated systems on the performance of organic electrodes [1-8]. Such analogues induce high redox activity due to their reversible switching between aromaticity and antiaromaticity across different redox states. Solid 3D spaces created by a subtle balance between structural flexibility and rigidity, along with molecular π-delocalization, are sufficient to stabilize the total electronic configuration of the stationary electrode molecules and to facilitate the frequent permeability of mobile electrolyte ions [8]. Thermodynamically durable and kinetically rapid redox interconversions serve as practical secondary organic batteries to further refine the battery technologies by leveraging strong metal chelation and immense ion permeability. This presentation discusses the capabilities of dual-ion battery technology for achieving high energy and power densities in utilizing porphyrinoid analogues and the exploratory direction.

REFERENCES

1. J.-Y. Shin, T. Yamada, H. Yoshikawa, K. Awaga, H. Shinokubo, *Angew. Chem. Int. Ed.* 2014, **53**, 3096.
2. J.-Y. Shin, Z. Zhang, K. Awaga, H. Shinokubo, *Molecules* 2019, **24**, 2433.
3. J. Hwang, K. Matsumoto, R. Hagiwara, H. Shinokubo, J.-Y. Shin, *Mater. Adv.* 2021, **2**, 2263.
4. J. Hwang, K. Matsumoto, R. Hagiwara, S.-Y. Liu, J.-Y. Shin, *Small Methods* 2022, **6**, 2101181.
5. S. Zhang, J. Hwang, Q. Phung, K. Matsumoto, R. Hagiwara, J.-Y. Shin, *Adv. Energy Mat*. 2023, **13**, 2301443.
6. S. Zhang, J. Hwang, Q. Phung, K. Matsumoto, R. Hagiwara, J.-Y. Shin, *Batteries & Supercaps* 2024, **7**, e202400004.
7. J. Hwang, S. Zhang, K. Matsumoto, J.-Y. Shin, *Electrochem. Soc. Japan*, *in press*.
8. J. Hwang, K. Matsumoto, R. Hagiwara, S. Ukai, H. Shinokubo, J.-Y. Shin, *Batteries & Supercaps* 2021, **4**, 1605.

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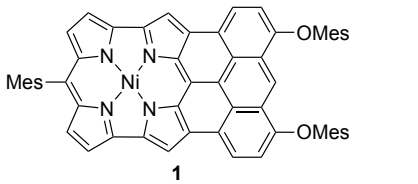


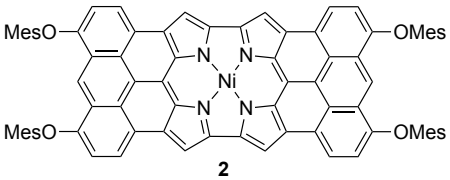
π-Expanded norcorroles as NIR absorbing dyes

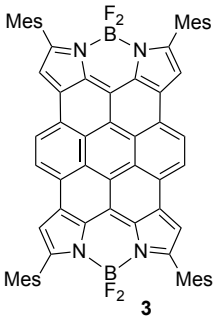
Hiroshi Shinokubo[a,b]

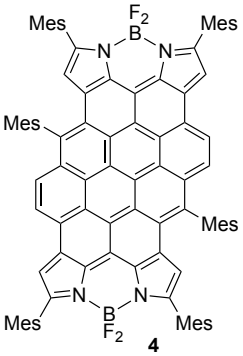
[a]*Department of Molecular and Macromolecular Chemistry, Graduate School of Engineering, Nagoya University*
[b]*Integrated Research Consortium on Chemical Sciences (IRCCS), Nagoya University*

Norcorrole, an antiaromatic porphyrinoid with a 16 π-electron system, consists of four pyrroles and two methine carbons. Due to the forbidden nature of their HOMO–LUMO transition, norcorrole derivatives generally exhibit weak and broad absorption bands in the near IR (NIR) region. Recently, we demonstrated that π-expansion of norcorroles, achieved through the fusion of aromatic π-systems, effectively enhances their NIR absorption property. We designed π-expanded norcorroles **1** and **2** with triply-fused anthracene units, which were synthesized through oxidative fusion of *meso*-anthrylnorcorroles.[1] Triply-fused mono- and dianthrylnorcorroles **1** and **2** exhibited near-infrared (NIR) absorption reaching 1900 nm. In addition, the bowl-shaped structure of these fused norcorroles enabled them to act as suitable receptors for C_{60}.
The molecular design was further extended to BODIPY-fused anthracene and anthanthrene **3** and **4**.[2] The antiaromatic character of these BODIPY-fused nanographenes **3** and **4** was corroborated by ^{1}H NMR analysis and ring current visualization. BODIPY dimers **3** and **4** exhibit narrow electrochemical HOMO–LUMO energy gaps as low as 0.84 eV and NIR absorption of up to 1600 nm. Due to the rapid decay profile of their excited state, BODIPY-fused nanographenes **3** and **4** **p**exhibit effective photothermal conversion efficiency. These results demonstrate that the BODIPY-fusion strategy effectively endows aromatic nanographenes with antiaromaticity and NIR absorption capability.









REFERENCES

1. K. Wang, A. Ghosh, D. Shimizu, H. Takano, M. Ishida, R. Kishi, H. Shinokubo, *Angew. Chem. Int. Ed.* **2025**, *64*, e202419289.
3. K. Wang, K. Isono, H. Takano, J. Oh, S. Kawakami, R. Sugimori, R. Kishi, D. Shimizu, S. Bhandari, M. Ishida, D. Kim, H. Shinokubo, *J. Am. Chem. Soc*. **2025**, *147*, 45441–45451.

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Probing and Expanding the Catalytic Scope of Cytochrome P450BM3 for Gaseous Alkane Hydroxylation through Decoy Molecule Strategies

Osami Shoji[a]

[a] *Department of Chemistry, Graduate School of Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, 464-8602, Japan E-mail: shoji.osami.w3@f.mail.nagoya-u.ac.jp*

ORALS

Cytochrome P450BM3 (P450BM3) from *Bacillus megaterium* is a highly efficient monooxygenase with great potential as a biocatalyst for green oxidation chemistry. However, its native catalytic activity is largely restricted to long-chain fatty acids, and wild-type P450BM3 is inactive toward small or non-native substrates such as aromatic compounds and gaseous alkanes. To overcome this limitation without relying on protein engineering, we developed a decoy molecule strategy in which chemically inert substrate analogues mimic native fatty acids to induce oxygen activation and formation of the reactive intermediate, Compound I. This approach enabled wild-type P450BM3 to catalyze the hydroxylation of various non-native substrates, including benzene and short-chain gaseous alkanes. Chemical evolution of decoy molecules led to second- and third-generation decoys based on N-acyl amino acids and amino acid dimers, which bind in the substrate access channel and enhance catalytic turnover. Some of these decoys also facilitated crystallization, allowing structural analysis of P450BM3 in catalytically relevant conformations. In whole-cell systems, catalytic efficiency depended strongly on decoy membrane permeability, and phenol production from benzene reached up to 59% GC yield using N-heptyl-L-prolyl-L-phenylalanine. Notably, we demonstrated for the first time that wild-type P450BM3 can catalyze the oxidation of methane to methanol using a chemically evolved decoy molecule (3CHPA-Pip-Phe) under 10 MPa methane pressure at ambient temperature.[1] Structural analysis revealed that the decoy molecule creates an enclosed cavity above the heme suitable for methane binding, and docking simulations supported the presence of multiple methane molecules near the active site. Furthermore, by combining the decoy strategy with directed evolution, we established a P450BM3-based system that utilizes bacterial quorum-sensing molecules as functional decoys. A fifth-generation mutant responsive to C10-homoserine lactone achieved efficient benzene hydroxylation without external decoy addition.[2] In addition, using a whole-cell biocatalytic system, we successfully achieved highly efficient propane hydroxylation while enabling recycling of *E. coli* cells, demonstrating the robustness and practical applicability of this approach for gaseous alkane oxidation.[3] Overall, decoy molecule strategies provide a powerful framework for expanding the catalytic scope of P450BM3, enabling sustainable and programmable oxidation of gaseous alkanes and other abiological substrates.

REFERENCES

(1) Ariyasu, S.; Yonemura, K.; Kasai, C.; Aiba, Y.; Onoda, H.; Shisaka, Y.; Sugimoto, H.; Tosha, T.; Kubo, M.; Kamachi, T.; et al. *ACS Catalysis* **2023**, *13* (13), 8613-8623. DOI: 10.1021/acscatal.3c01158.(2) Yokoyama, Y.; Ariyasu, S.; Karasawa, M.; Kasai, C.; Aiba, Y.; Sugimoto, H.; Shoji, O. *ChemCatChem* **2025**, *17* (1), e202401641. DOI: https://doi.org/10.1002/cctc.202401641.(3) Sugai, Y.; Karasawa, M.; Shoji, O. *JACS Au* **2025**, *5* (9), 4196-4203. DOI: 10.1021/jacsau.5c00453.

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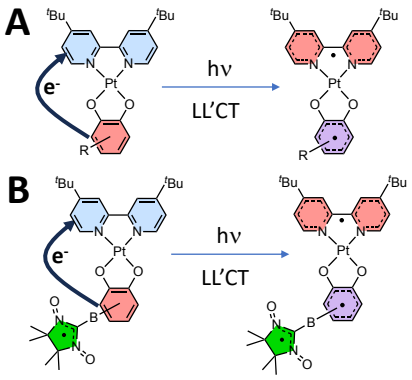
Exchange Coupling and Spin Relaxation in Ground State Analogs of Ligand-to-Ligand Charge Transfer Excited States

David A. Shultz[a], Anil Reddy Marri[a], Andre Nogueira[a], and Martin L. Kirk[b]

[a]*Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204*
[b]*Department of Chemistry and Chemical Biology, The University of New Mexico, MSC03 2060, 1 University of New Mexico, Albuquerque, NM 87131-0001*

ORALS

Photoinduced electron spin polarization (ESP)[1] remains a topic of intense study due to interest in molecule-based quantum information science.[2] ESP can be achieved by photoinitiated excited state intersystem crossing of organic chromophores and resultant polarization of covalently attached stable radicals.[3] Our groups have been interested in the photophysics and spin polarization capacity of ligand-to ligand charge transfer (LL'CT) complexes, ***Fig. A***.[4] We have reported photoinduced ESP of a stable radical covalently attached to the donor fragment (*e.g.*, catecholate, CAT, ***Fig. B***). In the molecule's ground state, the radical is a well-defined $S = ½$ specie possessing isotropic spin Hamiltonian parameters. However, upon irradiation of the CAT → diimine CT band, a three-spin LL'CT excited state is created with two chromophoric spins bridged by a diamagnetic heavy Pt(II) ion.



To date, these LL'CT excited states have avoided detection by transient electron paramagnetic resonance spectroscopy presumably due to large zero-field splitting (ZFS) and/or short spin-lattice relaxation times. Herein, we describe the preparation and characterization of a two-spin ground-state analog of the LL'CT excited state shown in ***Fig. A***. We compare and contrast ground- and excited state exchange coupling (also a topic of recent interest), spin Hamiltonian parameters, and magnetic relaxation, and relate our results to photoinduced ESP of the complexes in ***Fig. B***.

REFERENCES

1. Eills, J., et al., *Spin Hyperpolarization in Modern Magnetic Resonance.* Chem. Rev., 2023. **123**(4): p. 1417-1551.

2. Wasielewski, M.R., et al., *Exploiting chemistry and molecular systems for quantum information science.* Nat. Rev. Chem., 2020. **4**: p. 490-504.

3. Quintes, T., M. Mayländer, and S. Richert, *Properties and applications of photoexcited chromophore–radical systems.* Nat. Rev. Chem., 2023. **7**: p. 75-90.

4. Shultz, D.A., et al., *Bridge Connectivity Effects on Photoinduced Ground-State Electron Spin Polarization.* J. Chem. Phys., 2025. **162**: p. 084304.

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One-pot Porphyrin Metal-Organic Frameworks

Anna Sinelshchikova [a,b], Roberto Fernández de Luis [a], Stefan Wutteke [c], Jacopo Andreo [a]

[a] *BCMaterials, Basque Center for Materials, Applications and Nanostructures, 48940 Leioa, Spain*
[b] *Ikerbasque, Basque Foundation for Science, 48009, Bilbao, Spain*
[c] *Academic Centre for Materials and Nanotechnology, AGH University of Krakow, 30-055 Krakow, Poland*

ORALS

Porphyrin-based metal–organic frameworks (pMOFs) provide an attractive platform for the precise organisation of tetrapyrrole chromophores, enabling systematic control over their accessibility, coordination environment, and physicochemical properties. The rich photophysical and electrochemical behaviour of porphyrinoids makes them particularly appealing functional linkers for catalysis, sensing and biomedical applications[1, 2]; however, the multistep synthesis and purification of porphyrins remain a key bottleneck for the scalable preparation of pMOFs.
In this work, we present a one-pot synthetic strategy for pMOFs that integrates porphyrin formation by Adler-Longo method and MOF assembly under compatible reaction conditions. The approach relies on inexpensive precursors, such as pyrrole and aryl aldehydes, and eliminates the need for porphyrin isolation, substantially reducing synthetic complexity and cost. The crystallisation of MOF serves as a linker purification step and formation of the functional material at the same time. Using this method, we access pMOFs incorporating diverse porphyrins, including tetra(4-carboxyphenyl)porphyrin and tetra(3-carboxyphenyl)porphyrin, and demonstrate its compatibility with diverse inorganic nodes including Zr(IV) and Fe(III).
The optimised one-pot conditions allow the formation of highly crystalline and porous materials (Figure 1). The resulting porphyrin frameworks retain large accessible surface areas, with PCN-224 analogues reaching BET values of up to 1400 $m^2 g^{-1}$. Detailed structural characterisation reveals a higher defectivity of one-pot materials which can be exploited as an advantage for the absorption of large molecules.

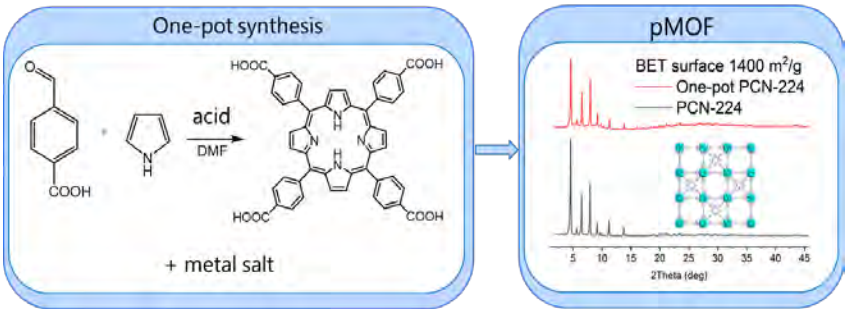


Figure 1. Scheme of the pMOFs one-pot synthesis. Comparison of PXRD of one-pot and conventional PCN-224.

These results highlight how simple reagents can be directly translated into well-defined porous porphyrin-based architectures, opening the way to large-scale applications of pMOFs. Fine-tuning the structure of the starting aldehydes and the metals present in the synthesis enables access to various systems that incorporate different metals both as porphyrin centres and as structural framework nodes. In summary, the one-pot method represents a versatile platform for obtaining both known and new pMOFs in a more cost-effective manner, enabling systematic exploration of how porphyrin structure and framework environment jointly govern material properties.

REFERENCES

1. X. Zhang, M. C. Wasson, et al. Coordination Chemistry Reviews. 2021, 429, 213615
2. Yu. G. Gorbunova, Yu. Yu. Enakieva, et al. Russian Chemical Reviews. 2022, 91, RCR5038

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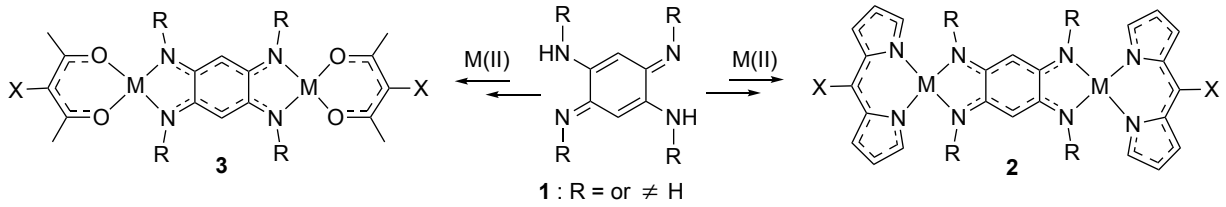
Dipyrromethene as ancillary ligand in coordination chemistry

Olivier SIRI

Aix-Marseille Université, CINaM, UMR 7325 CNRS, Campus de Luminy, case 913, F-13288 Marseille cedex 09, France.
E-mail: olivier.siri@univ-amu.fr

ORALS

A key challenge in the design and development of new ligands in coordination chemistry lies in controlling the π-electron distribution within the ligand framework. 2,5-Diamino-1,4-benzoquinonedimine **1** is a long-known compound, first reported in 1887 [1], yet it has remained largely unexplored due to its poor solubility and limited stability in solution. We have chosen to revisit the chemistry of compound **1** with the aim of developing new polynuclear complexes, which are of considerable interest for a wide range of technological applications. Our approach relies on the rich and adaptable coordination behavior of **1** in solution [2] and on metallic surfaces [3], which can be modulated by varying the nature of the N-substituents, as well as by exploiting the influence of ancillary ligands [4]. In particular, we have recently focused on the use of dipyrromethenes as an ancillary ligand in complexes of type **2**, owing to their structural flexibility and strong metal-binding ability.



Their electronic and steric properties was finely adjusted through substitution at the *meso*-position, enabling precise control over steric hindrance and electronic effects. The presentation will demonstrate that this tunability facilitates the design of metal complexes **2** with tailored optical and redox properties, that will be compared with those observed in the related compounds **3** bearing acac moieties [5].

REFERENCES

1. R. Nietzki, E. Hagenbach, *Ber. Dtsch. Chem. Ges.* **1887**, *20*, 328.
2. a) H. Audi, Z. Chen, A. Charaf-Eddin, A. D'Aléo, G. Canard, D. Jacquemin O. Siri *Chem. Commun.* **2014**, *50*, 15140. b) S. Pascal, O. Siri *Coord. Chem. Rev.* **2017**, 350, 178. c) Z. Chen, G. Canard, D. Jacquemin, C. Bucher, M. Giorgi, O. Siri *Inorg. Chem.*, **2018**, *57*, 12536. d) L. Pasquini, S. Mustefa Beyan, A. Khamidov, V. Jubault, T. Munteanu, G. Canard, P. Knauth, O. Siri *Eur. J. Inorg. Chem.* **2025**, *28*, e202400649.
3. a) V. M. Santhini, C. Wäckerlin, A. Cahlik, M. Ondráček, S. Pascal, A. Matěj, O. Stetsovych, P. Mutombo, P. Lazar, O. Siri, P. Jelinek *Angew. Chem. Int. Ed*. **2021**, 60, 439-445. b) A. Cahlík, J. Hellerstedt, J. I. Mendieta-Moreno, M. Švec, V. M. Santhini, S. Pascal, D. Soler-Polo, S. I. Erlingsson, K. Výborný, P. Mutombo, O. Marsalek, O. Siri, P. Jelínek *ACS Nano* **2021**, *15*, 10357–10365. c) A. Cahlík, M. Ondráček, C. Wäckerlin, A. Pinar Solé, O. Siri, M. Švec, P. Jelínek *ACS Nano* **2024**, *18*, 9576. d) A. Jiménez-Martín, T. Munteanu, Q. Chen, S. Pascal, A. Tintaru, B. Mallada, P. Mutombo, O. Siri, P. Jelínek, B. de la Torre *Mater. Chem. Front.* **2025**, *9*, 838.
4. O. Siri, J.-p. Taquet , J.-P. Collin, P. Braunstein *Dalton Trans*, **2007**, 148.
5. V. Jubault, D. Jacquemin, O. Siri, G. Canard, **2026** *submitted*.

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Influence of the distal His and the intramolecular disulfide Cys46-Cys55 bridge on the sulfide binding to human neuroglobin

Federico Sebastiani[a], Laura Cesati[a], Mirco Meglioli[b], Marco Borsari [b], Gianantonio Battistuzzi [b], Giulietta Smulevich[a]

[a]*Department of Chemistry "Ugo Schiff" DICUS, University of Florence, Via della Lastruccia 3, 50019 Sesto Fiorentino (FI), Italy*
[b]*Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia, Via Campi 103, 41125 Modena, Italy*

ORALS

Human neuroglobin (hNgb), found in the central and peripheral nervous systems, is overexpressed under hypoxic conditions induced by cerebral ischemia to protect neurons from damage [1, 2]. Recently, it has been suggested that the acid environment may favor the reaction of ferric Ngb with sulfide, producing a tightly bound complex [3]. Since H_2S is increasingly recognized as an important signalling molecule in the cardiovascular and nervous systems [4], it is crucial to understand the molecular mechanisms by which H_2S interacts with target proteins. hNgb contains a 6-coordinated low-spin heme since both the distal (His64) and proximal (His96) coordination positions of the heme iron are occupied by His residues and is characterized by rotational disorder [5,6]. Therefore, the Fe-exogenous ligand binding is modulated by the dissociation of the distal His [3]. Furthermore, the intramolecular disulfide bridge between Cys46 and Cys55 plays an important role in regulating the protein's activity and stability. Its cleavage strengthens the bond between the heme iron and the distal His, therefore, controlling exogenous ligand binding [7]. We have studied the reaction of H_2S with wild-type hNgb, its variant C46AC55A, in which the disulfide bridge has been eliminated, and the distal variants H64A and H64AK67A, to assess the role of the disulfide bridge and distal His in sulfide binding. We do not observe any appreciable effect of H-bonding on the iron-bound sulfide, as previously reported for Mb [8], with the Fe-S stretching wavenumbers of the hNgb-WT, its H64A, and H64AK67A variants very similar. As previously proposed [9], a distal side aromatic ring electrostatic interaction may stabilize the bound sulfide. Furthermore, a strengthened H-bond between the propionyl groups of the heme and nearby polar amino acid side chains, due to a rearrangement of the propionate groups, is envisaged. The lack of the Cys46-Cys55 disulfide bridge makes sulfide binding more difficult than in the WT, as the proteins are readily reduced by the H_2S, since the exogenous ligand is easily photolyzed under the laser beam. Unexpected was the finding that H_2S also induces reduction of heme, forming sulfheme derivatives, at both pH 7.4 and pH 10. These species are not detected in the distal mutants since the distal His is crucial for sulfheme complex formation [10]

REFERENCES

1. R.C. Li, S.Z. Guo, S.K. Lee, D. Gozal, *J Cereb Blood Flow Metab,* vol. 30, 2010, pp. 1874-1882.
2. L. Ciccone, S. Nencetti, S. Socci, E. Orlandini, *Neural Regen Res,* vol. 16, 2021, pp. 2353-2358.
3. T. Brittain, Y. Yosaatmadja, K. Henty, *IUBMB Life,* vol. 60, 2008, pp. 135-138.
4. C. Szabo, *Nat Rev Drug Discov,* vol. 6, 2007, pp. 917-935.
5. M. Meglioli, F. Sebastiani, M. Bellei, G Di Rocco, et al., *Inorg Chem* (2025), 64, 9066-9083.
6. M. Meglioli, L. Cesati, G. Battistuzzi, M. Borsari, et al., *Spectrochim. Acta Part A* (2026), in press.
7. M. Bellei, C.A. Bortolotti, G. Di Rocco, M. Borsari, et al., *J. Inorg. Biochem.,* vol. 178, 2018, pp. 70-86.
8. T. Bostelaar, V. Vitvitsky, J. Kumutirna, B.E. Lewis, et al., *J Am Chem Soc,* vol. 138, 2016, pp. 8476-848.
9. M.Rizzi, J.B. Wittenberg, A. Coda, M. Fasano, et al., *J Mol Biol,* vol. 244, 1994, pp. 86-99.
10. E. Roman-Morales, R. Pietri, et al., *Biochem. Biophys. Res. Commun.*, vol. 400, 2010, pp. 489-492.

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Synthesis of new derivatives of purpurin imide with functional group for PDT application.

Vincent SOL[a], **Luce Janice NDZIMBOU**[a], **Frédérique BREGIER**[a]

[a]*LABCiS UR22722, Univ. Limoges F-87000 Limoges, France*

Chlorins are among the most interesting photosensitizers for photodynamic therapy because they exhibit high quantum yield of the singlet oxygen generation and absorbance in the near infrared. Indeed the penetration depth of light into skin increases with wavelength from the UV to the near-infrared light range. Even if chlorins can be synthesized, they are present in the nature and the most abundant natural chlorin is the chlorophyll. After aceton extraction of chlorophyll a from *spirulana maxima*, it is possible to synthesize a derivative, the purpurin 18, which has an absorbance around 700 nm thanks to an additional anhydride exocyclic ring compared to the chlorin p6 whose maximum absorbance wavelength is at 650 nm.[1] The disadvantage is that this anhydride exocyclic ring is very reactive and can be easily opened by a nucleophile to lead to a derivative of chlorin p6. To preserve a cycle and thus the absorbance around 700 nm, previous work have shown that it is possible to open purpurin 18 with an amine and to recyclize to lead to purpurin imide derivatives which have also shown very important phototoxicity.[2] In this work we have therefore synthesized differents derivatives of purpurine imide, which have different reactive functional groups such as amino, sulfhydryl, maleimide, azide and alkyne to allow subsequent functionalization and open up the possibilities of using them . The structures of all new derivatives of purpurine imide were characterized by NMR and UV/visible spectroscopy and mass spectrometry.[3]

ORALS

REFERENCES

1. Drogat, N.; Barrière, M.; Granet, R.; Sol, V.; Krausz, P. High Yield Preparation of Purpurin-18 from Spirulina Maxima. *Dyes and Pigments* **2011**, *88* (1), 125–127. https://doi.org/10.1016/j.dyepig.2010.05.006.
2. Nazarova, A. I.; Feofanov, A. V.; Karmakova, T. A.; Sharonov, G. V.; Plyutinskaya, A. D.; Yakubovskaya, R. I.; Lebedeva, V. S.; Mironov, A. F.; Maurizot, J.-C.; Vigny, P. Effect of Substituents on Photochemical and Biological Properties of 13,15-N-Cycloimide Derivatives of Chlorin P6. *Russ J Bioorg Chem* **2005**, *31* (5), 482–494. https://doi.org/10.1007/s11171-005-0066-9.
3. Ndzimbou, L.J. ; Champavier, Y. ; Brégier, F. ; Sol, V. From Purpurin-18 to new purpurin imide derivatives with functional groups. *Journal of Porphyrins & Phthalocyanines* **2025**, 29, 454-466) https://doi.org/10.1142/S1088424625500385

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Porphyrin-Centered Photophysics and Electron-Transfer Strategies for Efficient TiO_2-Mediated Carbon Dioxide Reduction

Min-Jong Bong,[ab] Seung-Hwan Cha,[ab] Sangheon Jeong,[ab] Chul Hoon Kim,[ab] and Ho-Jin Son[ab]

[a]*Department of Advanced Materials Chemistry, Korea University, Sejong 30019, Republic of Korea*
[b]*Division of Smart Energy Convergence Engineering, Korea University, Sejong 30019, Republic of Korea*

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Porphyrins provide an exceptionally tunable molecular platform for artificial photosynthesis owing to their intense visible-light absorption, diverse redox chemistry, and modular structural design. These characteristics allow porphyrins to function not only as chromophores but also as electronic and catalytic control elements within dye-sensitized TiO_2 systems.[1] Building on this versatility, we examined how monomeric Zn-porphyrins, π-extended porphyrin oligomers, and porphyrinic frameworks shape interfacial electron-transfer (ET) processes that govern photochemical CO_2 reduction.[2-5] The extended conjugation of porphyrin oligomers and MOF-based porphyrin arrays promotes rapid exciton delocalization and directional energy migration, thereby enhancing charge delivery to the molecular catalyst or TiO_2-immobilized catalytic site even when excited-state energies are relatively low.[4,5] These photophysical advantages seamlessly translate into more efficient sensitization because the bulk TiO_2 support provides low-lying trapping sites capable of accepting electrons through both direct injection and long-lived collisional ET from solution-phase porphyrin radicals. Thus, the intrinsic excited-state behavior of porphyrins and the ET landscape of TiO_2 converge to create a cooperative charge-transport environment. On the other hand, extending this porphyrin-centered design to catalysis, TiO_2-anchored porphyrins (M-TCPP; M = Fe, Co, Ni, Cu) exhibit markedly enhanced stability and reactivity. Strong surface coupling suppresses porphyrin dimerization and stabilizes metal-based intermediates, enabling Fe/Co/Ni porphyrins to reach CO turnover numbers above 3000, while Cu-TCPP follows a distinct Cu–H pathway favoring H_2 evolution. Together, these results demonstrate that rational modulation of porphyrin photophysics and interfacial ET provides a unified blueprint for designing durable, selective, and high-performance molecular CO_2-reduction systems.

REFERENCES

1. H.-J. Son,* C. Pac, and S. O. Kang *Acc. Chem. Res.* **2021**, *54*, 4530-4544.
2. D.-I. Won, J.-S. Lee, Q. Ba, Y.-J. Cho, H.-Y. Cheong, S. Choi, C. H. Kim,* H.-J. Son,* C. Pac, and S. O. Kang* *ACS Catal.* **2018**, *8*, 1018-1030.
3. S. Choi, C. H. Kim, J.-O. Baeg, H.-J. Son,* C. Pac, and S. O. Kang* *ACS Appl. Energy Mater.* **2020**, *3*, 11581-11596.
4. S. Choi, W.-J. Jung, K.-T. Park, S.-Y. Kim, J.-O. Baeg, C. H. Kim,* H.-J. Son,* C. Pac, and S. O. Kang* *ACS Appl. Mater. Interfaces* **2021**, *13*, 2710-2722.
5. S. Choi, M. S. Choe, D. Lee, J. Y. Shin, and H.-J. Son* *ACS Appl. Energy Mater.* **2024**, *7*, 3602-3617.

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Chiral ruthenium phthalocyanine for highly efficient dia- and enantioselective catalysis

A. B. Sorokin[a], **A. P. Kroitor**[a,b], **A. A. Dmitrienko**,[b] **A. G. Martynov**,[b] **Yu. G. Gorbunova** [b,c]

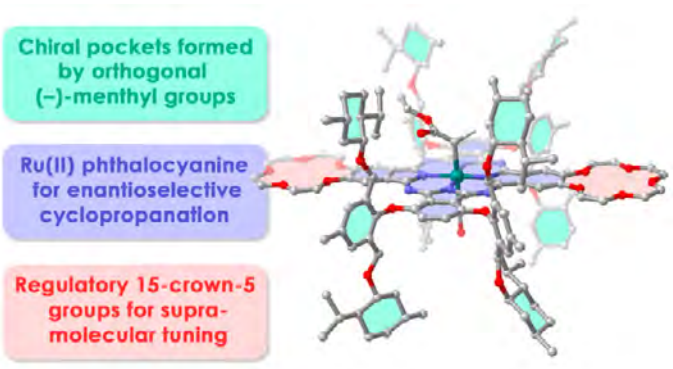
[a]*Institut de Recherches sur la Catalyse et l'Environnement de Lyon, IRCELYON, CNRS - Université Lyon 1, Villeurbanne, France*
[b]*Frumkin Institute of Phisycal Chemistry and Electrochemistry, Russian Academy of Sciences, Moscow, Russia*
[c]*Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow, Russia*

ORALS

Metal phthalocyanine complexes (MPc) are effective catalysts for a variety of reactions [1]. However, their use in chiral catalysis remains extremely rare despite the fact that numerous chiral MPc have been prepared [2]. This paradox can be explained by the remote position of chiral substituents at the macrocycle periphery, far from the catalytic metal site, and their location in the plane of tetrapyrrolic core that prevents efficient asymmetric induction in enantioselective reactions.

Addressing this challenge, we have prepared unprecedented chiral RuPc* with chiral motifs near the catalytic metal site by cross condensation of the chiral 3,6-bis-aryloxyphthalonitrile bearing two (1*R*,2*S*,5*R*)-mentoxy groups orthogonal to the aromatic plane and (15-crown-5)phthalonitrile [3]. Four complexes containing chiral menthyl groups (**M**) and 15-crown-5 units (**C**), notably **RuPc[MC$_3$](CO)**, **RuPc[*opp*-M$_2$C$_2$](CO)**, **RuPc[*adj*-M$_2$C$_2$](CO)** and **RuPc[M$_3$C](CO)**, were isolated in pure form and fully characterized by UV-Vis, circular dichroism, HRMS, various ^{1}H NMR and ^{13}C NMR techniques. Their evaluation in the benchmark asymmetric cyclopropanation reaction of styrene derivatives by ethyl diazoacetate indicated that **RuPc[*opp*-M$_2$C$_2$](CO)** complex was the most efficient in terms of diastereo- and enantioselectivity.

The study revealed the strong dependence of the stereoselectivity on the solvent nature and salt additives, which caused conformational changes of the flexible chiral surrounding as evidenced by multinuclear NMR and CD spectra. Upon moving from commonly used CH_2Cl_2 to EtOH with the addition of $NaPF_6$ a significant enhancement of enantioselectivity (from 35 % to 84 % with *p*-methylstyrene) was observed. Of particular importance is a very high diastereoselectivity of cyclopropanation promoted by the incorporation of sodium cations into crown ether cavities of phthalocyanine to attain *trans/cis* ratio up to 499:1. Such a regulating effect in chiral catalysis involving tetrapyrrolic complexes has not been previously observed, rendering this complex as a prominent example of the phthalocyanine tunable catalyst.



REFERENCES

1. A. B. Sorokin, *Chem. Rev.*, **2013**, *113*, 8152.
2. H. Lu, N. Kobayashi, *Chem. Rev.*, **2016**, *116*, 6184.
3. A. P. Kroitor, A. A. Dmitrienko, G. A. Kirakosyan, C. Lorentz, A. G. Martynov, Y. G. Gorbunova, A. Y. Tsivadze, A. B. Sorokin, *ACS Catal.*, **2025**, *15*, 4984.

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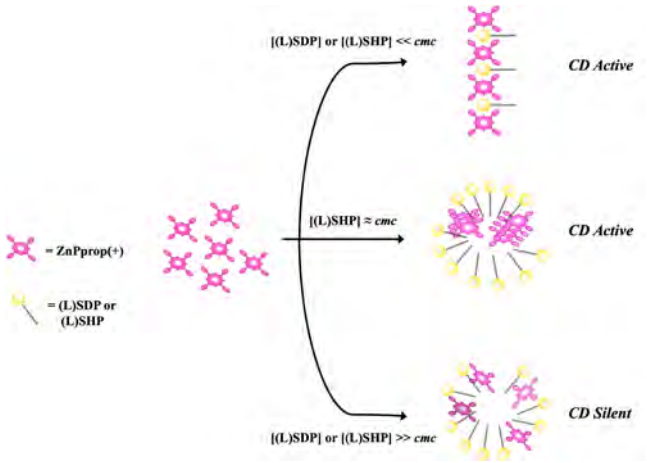
Supramolecular Chirogenesis in Porphyrin-Surfactant Based Heterosystems

Manuela Stefanelli[a], Giuseppe Pomarico[b], Mariano Venanzi[a], Roberto Paolesse[a], Donato Monti[b]

[a]*Department of Chemical Science and Technologies, University of Rome Tor Vergata, Italy*
[b]*Department of Chemistry, Sapienza University of Rome, Italy*

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The assembly behavior of porphyrins in the presence of surfactants has long been studied with the goal of developing artificial enzymes and photodynamic therapy drugs. The interactions between porphyrins and surfactants are highly sensitive to their specific characteristics, as well as to factors such as concentration, ratio, and the properties of the assembly medium, including ionic strength, temperature, and pH. Within these systems, various intermolecular interactions—namely porphyrin–porphyrin, porphyrin–surfactant, and surfactant–surfactant—compete with one another. The formation of surfactant–porphyrin complexes is favored when porphyrin-surfactant interactions are predominant. By carefully selecting appropriate porphyrin-surfactant pairs and adjusting the conditions, it is possible to create hetero-assembled structures in which porphyrin platforms can exist as either aggregates or monomers. This general approach can be leveraged to construct chiral porphyrin-surfactant systems by utilizing chiral surfactants as "chiral effectors" for supramolecular chirogenesis. In this contribution, we present our recent findings on the transfer of chirality from chiral surfactants—specifically, the sodium salts of dodecyl and hexadecyl amidic derivatives of proline (SDP and SHP)—to an amphiphilic, achiral porphyrin (ZnPprop(+)). We explore various surfactant concentrations, both above and below the critical micellar concentration (*cmc*) [1]. Our results indicate that the alkyl chains of the surfactant molecules play a significant role in determining macrocycle inclusion and the efficiency of chirality transfer, emphasizing that the hydrophobic effect is the primary driving force behind this process. At the same time, metal coordination and electrostatic forces are crucial for the supramolecular chirogenesis process.



REFERENCES

1. P. Sbardella, M. Stefanelli, G. Pomarico, C. Bombelli, F. Ceccacci, R. Paolesse, M. Venanzi, D. Monti *Int. J. Mol. Sci.* **2025***, 26(23),* 11330.

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Quantifying the electronic properties of tetrapyrroles: Predicting spectral properties from the electronic structures

Martin J. Stillman

Department of Chemistry, The University of Western Ontario, London, Canada

The very rich spectroscopic and redox properties of tetrapyrroles underpin the natural and technological uses of these molecules. The metalated protoporphyrin IX variants in heme proteins and the magnesium chlorins in chlorophylls are wonderful examples from natural chemistry. The properties of just these two families depend directly on their electronic structures as tuned by the biological environment. The properties of the phthalocyanines drive extensive technological applications that again depend on how the specific metal used, and their oxidation and spin states, together with electronically-active peripheral groups and the degree of aggregation, modify the underlying electronic structures of the tetrapyrrole ring scaffold. Quantifying this range of functions has been a challenge for many decades being based on the interpretation of the electronic origins of a wide range of redox and spectroscopic data. However, use of ever more sophisticated computational approaches had led to successes. Quantification brought the opportunity for modelling properties and then predicting properties of novel structures. With detailed absorption, emission, and magnetic circular dichroism spectral data, we can characterize the specific electronic effects from the molecular tuning of tetrapyrroles. By connecting individual properties to parameters in the electronic structure (through trend lines) we can identify the electronic structural properties required for a desired property. This led us from the analysis of the Zn-phthalocyanine spectra of the 1970s and 1980s (1), to the trend lines of 2005 (2), and to the predictions in 2017 (3), and then to today, where we can use the predictions of the electronic structure to guide molecular design.

REFERENCES

1. MJ Stillman, and T Nyokong. “Absorption and magnetic circular dichroism spectral properties of phthalocyanines. Part 1: complexes of the dianion Pc (-2)”. Phthalocyanines: properties and applications. 1989;1:133-289.
2 J Mack, Y Asano, N Kobayashi and MJ Stillman “Application of MCD Spectroscopy and TD−DFT to a Highly Non-Planar Porphyrinoid Ring System. New Insights on Red−Shifted Porphyrinoid Spectral Bands”, J. Am. Chem. Soc. 2005, 127, 50, 17697–17711
3 A Zhang, L Kwan, and MJ Stillman “The spectroscopic impact of interactions with the four Gouterman orbitals from peripheral decoration of porphyrins with simple electron withdrawing and donating groups”, Org. Biomol. Chem., 2017,15, 9081-9094.

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Hydrolytic Scission of (Sub)porphyrazine Macrocycle as a New Approach to Diazatripyrrines

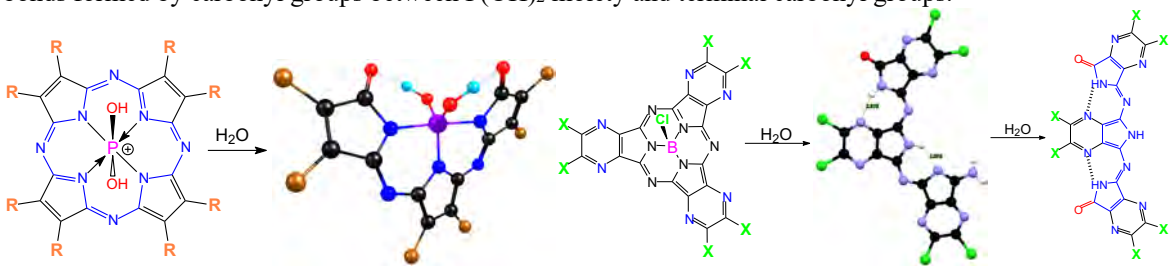
Pavel A. Stuzhin[a], **Dmitriy A. Lazovskii**[a], **Alina M. Fazlyeva**[a], **Ivan A. Skvortsov**[a]

[a]*Research Institute of Macroheterocycles, Ivanovo state University of Chemistry & Technology, RF-153000 Ivanovo, Russia*

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Introduction of electronegative non-metal atoms (B^{III}, Si^{IV}, P^{V}) in the central coordination cavity of the porphyrazine-type macrocycles decreases the electron density on the constituting atoms as compared to the corresponding metal complexes. In addition electron affinity of the macrocycle can be considerably enhanced by fusion of the electron deficient heterocycles (e.g. pyrazine or 1,2,5-thiadiazole rings) and/or peripheral halogenation. All these factors can increase the positive charge on the pyrrolic α-carbon atoms enabling nucleophilic attack on $C_{\alpha}=N_{meso}$ bonds. Thus, it was previously shown that phorphorus(V) phthalocyanines can bind reversibly alkoxide to one of the C_{α}-atoms [1].

We have demonsrated that P^{V} complexes of aryl substituted porphyrazines undergo hydrolytic scission of the macrocycle with formation of the diazitripyrrine-1,14-dione derivatives, stabilized by intramolecular hydrogen bonds formed by carbonyl groups between $P(OH)_2$ moiety and terminal carbonyl groups.



Hydrolysis of boron(III) complexes of electron deficient subporphyrazines containing fused pyrazine or perfluorinated benzene rings also leads to the scission of the macrocycle and deborylation with formation of the 14-aminodiazatripyrrine-1-one and finally to diazitripyrrine-1,14-dione derivatives [2]. Compounds with fused pyrazine rings are stabilized by intramolecular hydrogen bond between the pyrazine nitrogens in the central unit and pyrrolic NH groups.

Influence of fused rings, peripheral substituents non-metal atoms and possible mechanism of the hydrolytic scission of the macrocycle are discussed.

The support from Russian Science Foundation (grant 25-73-20126) is gratefully acknowledged.

REFERENCES

1. Kolomeychuk, F. M.; Safonova, E. A.; Polovkova, M. A.; Sinelshchikova, A. A.; Martynov, A. G.; ... & Gorbunova, Y. G. *J. Am. Chem. Soc.*, 2021, *143*, 14053-14058.
2. Fazlyeva, A. M.; Skvortsov, I. A.; Somov, N. V.; Stuzhin, P. A. *Inorganic Chemistry*, 2025, *64*, 19197–19206. DOI: 10.1021/acs.inorgchem.5c02123

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Precision synthesis of porphyrin-based supramolecular polymers

Kazunori Sugiyasu[a]

[a]*Department of Polymer Chemsitry, Kyoto University*

Supramolecular polymers are expected in a variety of applications; nevertheless, its synthetic methodology had remained unestablished. In 2014, we demonstrated living supramolecular polymerization, a method to control supramolecular polymerization in a way similar to living polymerization [1]. Since then, we have achieved a variety of mesoscopic supramolecular structures with controlled size and shape [2].
During the course of this study, we discovered a unique mesoscopic structure: concentric toroids (Figure 1) [3]. Mechanistic insight into the propagation of concentric toroids suggested that it involves secondary nucleation as a rate-determining step. With this understanding, we succeeded in the synthesis of multicomponenent concentric toroids, which can be considered as two-dimensional block polymers, with tailored composition and sequence [4].

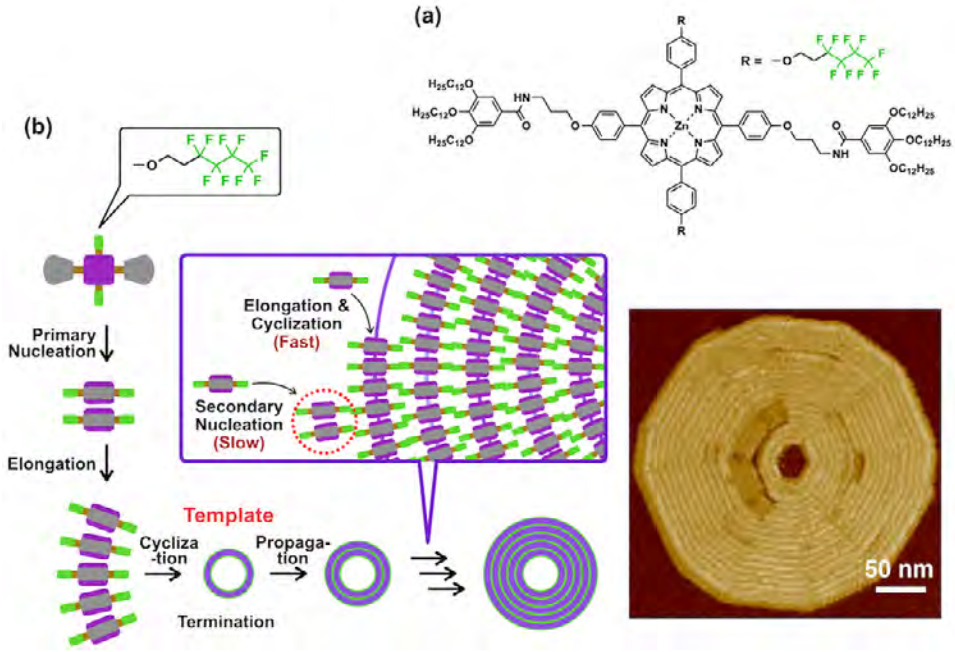


Figure 1. (a) Structure of a monomer used in this study; (b) Self-assembly mechanism of concentric toroids.

REFERENCES

1. S. Ogi, et al., *Nature Chem.* **2014**, *6*, 188.
2. K. Sugiyasu, *Polymer J.* **2021**, *53*, 865. [Account]
3. Sasaki, et al., *Nature Commun.* **2020**, *11*, 3578.
4. N. Sasaki et al., *Nature Chem.* **2023**, *15*, 922.

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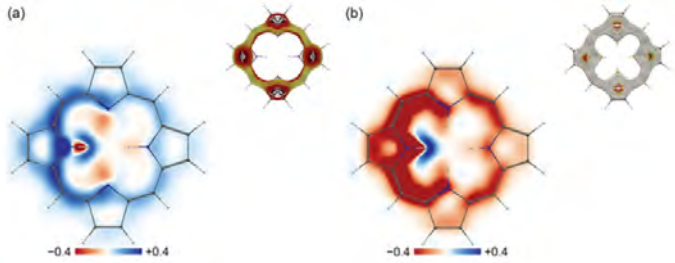
Magnetically Induced Current Densities and Nuclear Magnetic Shielding Tensors

Dage Sundholm, Daniel Blasco, Maria Dimitrova, Rinat T. Nasibullin, Qian Wang

Department of Chemistry, Faculty of Science, University of Helsinki, Helsinki, Finland

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An expression for calculating gauge-independent magnetically induced current density (MICD) susceptibilities is obtained by combining the commonly used second-derivative approach to calculate nuclear magnetic resonance (NMR) shielding tensors with the less well-known integral approach, whose integrand is called magnetic shielding density (MSD), *i.e.,* the spatial contribution to NMR shielding tensors.[1,2,3] Visualisation of the MSD and integration of atomic domains of it are used for understanding the spatial origin of the NMR shielding tensors. The degree of aromaticity can be determined by integrating the magnetically induced ring-current (MIRC) strength, which can be obtained by integrating the flux passing through a plane intersecting the ring or by line integration of the magnetic field in the centre of the ring vortex employing the Ampère-Maxwell law.[4] The MIRC strength and its tropicity reveal whether the molecular ring is aromatic, antiaromatic or non-aromatic. The MSD as well as the tropicity of the MICD,[5] the MIRC strength, and orbital contributions to the MICD[6] can be calculated with our gauge-including magnetically induced currents (GIMIC) method.[7,8] The methods are used in aromaticity studies of ring-shaped molecules as well as in MICD and MSD studies on general molecular structures.



The MSD and MICD of a) trans-porphin and b) isophlorin

REFERENCES

[1] D. Sundholm, M. Dimitrova, D. Blasco, ”Chapter 5: Magnetically Induced Current Densities and Nuclear Magnetic Shielding Constants, in Series New Developments in NMR, NMR Spectroscopic Parameters: Theories and Models, Computational Codes and Calculations”, Ed. G. A. Aucar, 2025 eBook Collection Royal Society of Chemistry 38 (2025) 170-204. 10.1039/9781837678020-00170

[2] H. Fliegl, M. Dimitrova, R. J. F. Berger, D. Sundholm, ”Spatial Contributions to ^{1}H NMR Chemical Shifts of Free-Base Porphyrinoids”, Chemistry 3 (2021) 1005-1021. 10.3390/chemistry3030072

[3] R. K. Jinger, H. Fliegl, R. Bast, M. Dimitrova, S. Lehtola, D. Sundholm, ”Spatial contributions to NMR chemical shifts”, J. Phys. Chem. A 125 (2021) 1778-1786. 10.1021/acs.jpca.0c10884

[4] R. J. F. Berger, M. Dimitrova, R. T. Nasibullin, R. R. Valiev, D. Sundholm, ”Integration of Global Ring Currents Using the Ampère-Maxwell Law”, Phys. Chem. Chem. Phys. 24 (2022) 624-628. 10.1039/D1CP05061C

[5] Q. Wang, J. Pyykkö, M. Dimitrova, S. Taubert, D. Sundholm ”Current-density pathways in figure-eight-shaped octaphyrins”, Phys. Chem. Chem. Phys. 25 (2023) 12469-12478. 10.1039/D3CP01062G

[6] R. T. Nasibullin, M. Dimitrova, R. R. Valiev, D. Sundholm, ”Orbital contributions to magnetically induced current densities using gauge-including atomic orbitals”, Chem. Sci. 16 (2025) 8040-8052. 10.1039/D5SC00627A

[7] J. Jusélius, J. Gauss, D. Sundholm, ”Calculation of Current Densities using Gauge-Including Atomic Orbitals”, J. Chem. Phys. 121 (2004) 3952-3963. 10.1063/1.1773136

[8] D. Sundholm, H. Fliegl, R. J. F. Berger, ”Calculations of Magnetically Induced Current Densities - Theory and Applications”, WIREs Comput. Mol. Sci. 6 (2016) 639-678. 10.1002/wcms.1270

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Chiroptical Properties of Inherently Chiral *N*-Alkyl Corroles

Ernesto Santoro[a], Francesco Pizzoli[b], Umberto Calice[a], Alessia Fata[b], Gabriele Magna[b], Sara Nardis[b], Roberto Paolesse[b], Stefano Superchi[a]

[a]*University of Basilicata, via dell'Ateneo Lucano, 10; 85100 Potenza, ITALY*
[b]*University of Rome Tor Vergata, via della Ricerca Scientifica; 00133 Rome, ITALY*

Corroles have recently gained increasing attention due to their peculiar chemistry[1] which has led to numerous applications in energy conversion, catalysis, medicinal chemistry, and chemical sensors. Moreover, the optimization of *N*-alkyl corroles synthesis unlocked the capability of coordination of divalent metals, such as Pd and Cu, previously forbidden by the corrole trianionic nature.[2,3] *N*-alkylation of corroles on either the N-21 and/or N-22, breaks the molecular symmetry, making the molecule chiral and stabilizing the macrocycle saddling into two enantiomerical inherently chiral structures. The enantiomers of free base and metal complexes of N-21 and N-22 mono- and di- methylated regioisomers of *meso*-tritolyl corrole were be separated by HPLC on chiral stationary phases and their their chiroptical properties, *i.e.* electronic circular dichroism (ECD) and circular polarized luminescence (CPL) investigated by TDDFT computations.[3] Such analysis provided a deep insight on the macrocycle conformational and electronic properties and allowed to establish a nonempirical correlation between the absolute configuration of the corrole and the ECD spectral features allied to the Soret region.

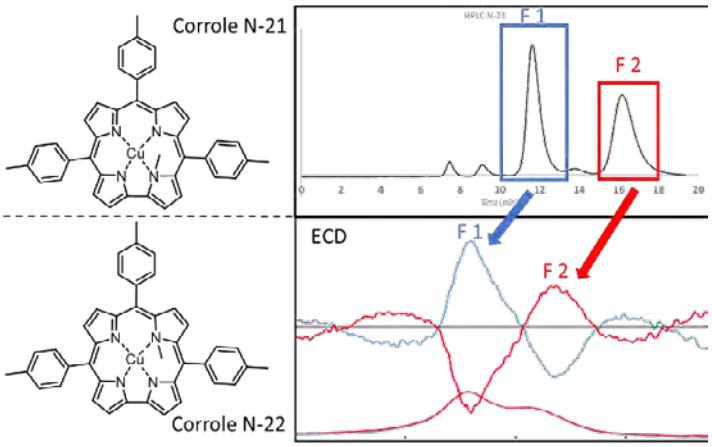


Figure 1

REFERENCES

1. Kumar, A.; Kim, D.; Kumar, S.; Mahammed, A.; Churchill, D. G.; Gross Z. *Chem. Soc. Rev.,* **2022**, *52*, 573.
2. Pizzoli, F.; Nardis, S.; Fata, A.; Marsotto, M.; Petrella, G.; Fronczek, F. R.; Smith, K. M.; Paolesse, R. *J. Porphyrins Phthalocyanines* **2024**, *28*, 358.
3. Pizzoli, F.; Mita, A.; Caroleo, F.; Nardis, S.; Calice, U.; Caporale, M.; Belviso, S.; Superchi, S.; Marconi, A.; Calvaresi, M.; Capolungo, C.; Prodi, L.; Smith, K. M.; Fronczek, F. R.; Paolesse, R. *Chem. Eur. J.* **2023**, *29*, e202302517.

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Insights into heme binding and transport in bacterial cytochrome *c* biogenesis

Molly C. Sutherland[a], **Alicia N. Kreiman**[a], **Tania Yeasmin**[b]

[a]*Department of Biological Sciences, University of Delaware, Newark, DE, USA*
[b]*Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, USA*

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Heme is a critical cofactor for key biological processes across all domains of life. This is due to heme's unique redox properties, which allow it to function in gas sensing, electron transfer, and the regulation of cellular processes. Heme's redox properties also render it highly cytotoxic, resulting in tight regulation of intracellular heme levels. Despite their critical importance, the mechanisms of heme trafficking and transport remain poorly understood. Here, we utilize the bacterial cytochrome *c* biogenesis pathways as model systems to probe mechanisms of heme trafficking. Cytochromes *c* are hemoproteins found in nearly all organisms that generally function in electron transport chains for cellular energy generation. Cytochromes *c* require the covalent attachment of heme for protein function. Heme attachment occurs outside the bacterial cell (in the periplasm). Therefore, heme must be transported from the site of synthesis inside the cell to the site of attachment outside the cell, where heme is then stereospecifically positioned for attachment to apocytochrome *c*. In bacteria, this process can occur via two pathways: System I (CcmABCDEFGH) or System II (CcsBA) (reviewed in [1]. We describe the biochemical mapping of the heme transport pathways for both System I (CcmCD) [2] and System II (CcsBA). Cysteine-heme crosslinking [3], a novel approach that exploits the formation of covalent bonds between a cysteine thiol and heme vinyl group, was used to identify residues that directly interact with heme. Mapping of these residues onto published cryo-EM structures of CcmCD [4] and CcsBA [5] delineates the heme channel in each pathway. We provide direct biochemical evidence for heme transport in Systems I and II of bacterial cytochrome *c* biogenesis. These results enable comparison of two heme transporters and provide insights into general mechanisms of heme trafficking.

REFERENCES

[1] R.G. Kranz, M.C. Sutherland, Mechanisms and Control of Heme Transport and Incorporation into Cytochrome c, Annual Review of Microbiology (2025). https://doi.org/10.1146/annurev-micro-050624-031631.

[2] A.N. Kreiman, S.E. Garner, S.C. Carroll, M.C. Sutherland, Biochemical mapping reveals a conserved heme transport mechanism via CcmCD in System I bacterial cytochrome *c* biogenesis, mBio 16 (2025) e03515-24. https://doi.org/10.1128/mbio.03515-24.

[3] M.C. Sutherland, J.M. Jarodsky, S. Ovchinnikov, D. Baker, R.G. Kranz, Structurally Mapping Endogenous Heme in the CcmCDE Membrane Complex for Cytochrome c Biogenesis, J. Mol. Biol. 430 (2018) 1065–1080. https://doi.org/10.1016/j.jmb.2018.01.022.

[4] J. Li, W. Zheng, M. Gu, L. Han, Y. Luo, K. Yu, M. Sun, Y. Zong, X. Ma, B. Liu, E.P. Lowder, D.L. Mendez, R.G. Kranz, K. Zhang, J. Zhu, Structures of the CcmABCD heme release complex at multiple states, Nat Commun 13 (2022) 6422. https://doi.org/10.1038/s41467-022-34136-5.

[5] D.L. Mendez, E.P. Lowder, D.E. Tillman, M.C. Sutherland, A.L. Collier, M.J. Rau, J.A.J. Fitzpatrick, R.G. Kranz, Cryo-EM of CcsBA reveals the basis for cytochrome c biogenesis and heme transport, Nat Chem Biol 18 (2022) 101–108. https://doi.org/10.1038/s41589-021-00935-y.

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Porphyrin–Polyoxometalate Molecular Hybrids as Highly Efficient, Durable, Visible-Light-Responsive Photocatalysts

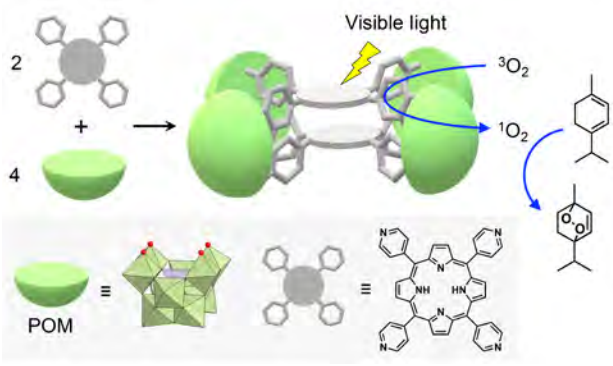
Kosuke Suzuki[a]

[a] *Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8561*

ORALS

Porphyrins are attractive photocatalysts because of their strong visible-light absorption and ability to generate reactive singlet oxygen ($^1O_2$) from molecular oxygen ($^3O_2$). However, their practical photocatalytic use is limited by poor durability, as porphyrin frameworks are readily decomposed by the generated $^1O_2$. Developing porphyrin-based photocatalysts that combine high activity and long-term stability therefore remains a critical challenge. Polyoxometalates (POMs) are structurally well-defined, bulky anionic metal-oxo clusters composed of early transition metals such as tungsten and molybdenum. Their rich redox chemistry, tunable electronic structures, and strong coordination ability make them versatile inorganic building units for functional hybrid materials, particularly when lacunary POMs act as multidentate ligands.[1-3]

In this study, we report porphyrin–POM molecular hybrids featuring stacked porphyrin dimers designed to achieve both efficient $^1O_2$ generation and enhanced durability.[4,5] The heavy atoms within the POM framework promote intersystem crossing from the photoexcited singlet to the triplet state, while the rigid hybrid architecture formed through POM coordination and porphyrin π–π stacking suppresses structural distortion of the porphyrin rings caused by $^1O_2$ addition. In addition, tuning the LUMO energy levels of the POM units enables control over the relaxation pathways from the photoexcited states of the porphyrin units, thereby facilitating efficient $^1O_2$ generation. The hybrids were synthesized by reacting lacunary POMs with 5,10,15,20-tetra(4-pyridyl)porphyrin in organic media. Single-crystal X-ray diffraction revealed well-defined structures in which two porphyrins are stacked and coordinated by four POM units, with tunable stacking geometries depending on the synthesis conditions. The resulting hybrids exhibited superior photocatalytic performance in visible-light-driven aerobic oxidation reactions. Compared with free porphyrins, the POM–porphyrin hybrids exhibited higher $^1O_2$ generation efficiency and markedly improved resistance to degradation. These results demonstrate that POM-based structural and electronic modulation provides an effective strategy for designing durable and highly active porphyrin photocatalysts.



REFERENCES

1. C. Li, N. Mizuno, K. Yamaguchi, K. Suzuki, *J. Am. Chem. Soc.* **2019**, *141*, 7687.
2. K. Yonesato, D. Yanai, S. Yamazoe, D. Yokogawa, T. Kikuchi, K. Yamaguchi, K. Suzuki, *Nat. Chem.* **2023**, *15*, 940.
3. K. Xia, T. Yatabe, K. Yonesato, S. Kikkawa, S. Yamazoe, A. Nakata, R. Ishikawa, N. Shibata, Y. Ikuhara, K. Yamaguchi, K. Suzuki, *Nat. Commun.* **2024**, *15*, 851
4. M. Yamaguchi, K. Shioya, C. Li, K. Yonesato, K. Murata, K. Ishii, K. Yamaguchi, K. Suzuki, *J. Am. Chem. Soc.* **2024**, *146*, 4549.
5. M. Yamaguchi, K. Yonesato, K. Shioya, C. Li, K. Murata, K. Ishii, K. Yamaguchi, K. Suzuki, *Chem. Sci.* **2025**, *16*, 9178.

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Synthesis of *meso*-Spiroadamantyl-Fused Calix[4]pyrroles and Derivatization of Calix[4]Pyrroles to Calix[4]phyrins

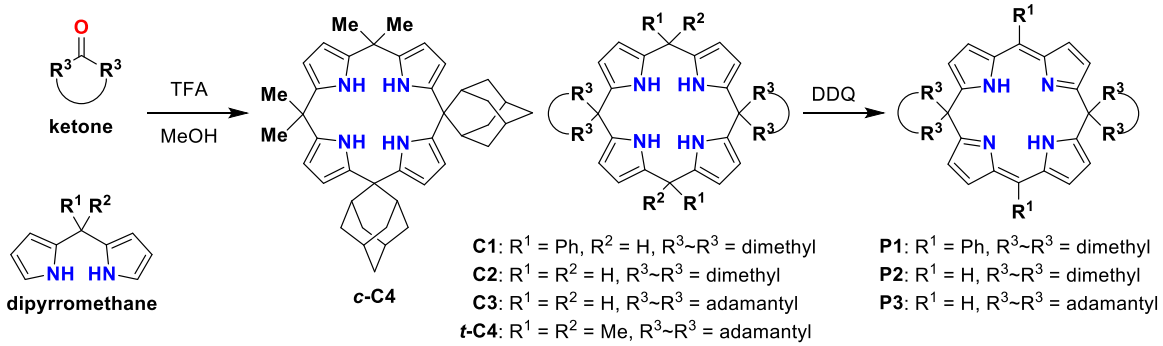
Masaaki Suzuki[a], **Yuzuki Tashiro**[b]

[a]*Graduate School of Natural Science and Technology, Shimane University*
[b]*Interdisciplinary Faculty of Science and Engineering, Shimane University*

ORALS

Calix[4]pyrroles, also known as porphyrinogens, are precursors of porphyrins and normally undergo further oxidation when the cyclic intermediates have hydrogen atoms at their *meso*-positions, resulting in the formations of fully oxidized macrocycles. Therefore, the isolation of calix[4]pyrroles with *meso*-hydrogen atoms is still problematic. When treated with a catalytic amount of trifluoroacetic acid, mixtures of 5-phenyl (R^1 = Ph, R^2 = H) or unsubstituted (R^1 = R^2 = H) dipyrromethanes and ketones (acetone or 2-adamantanone) in methanol gave, after recrystallisation from mixed solvents of dichloromethane and methanol, precipitates characterized as calix[4]pyrroles **C1**, **C2**, and **C3** with hydrogen atoms at the 10- and 20-positions. In the case of a combination of 5,5-dimethyldipyrromethane (R^1 = R^2 = Me) and 2-adamantanone produced a mixture of *cis*- and *trans*-derivatives ***c*-C4** and ***t*-C4** as a result of scrambling side reaction of the precursor or the intermediate, which were identified by slica-gel column separation and afore-mentioned subsequent X-ray crystalography for ***c*-C4**. Such products possessing *meso*-hydrogen atoms gradually disappeared in the solution state, probably due to oxidation.

The oxidative derivatization of such calix[4]pyrroles bearing *meso*-hydrogen atoms into the corresponding porphodimethenes **P1**, **P2**, and **P3** using 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) was also examined. Despite the minor electronic differences between the dimethyl and 2-adamantly substituents, the reaction to produce **P2** took a longer period than for **P3** and the color of the **P3** solution was apparently different from that of **P2**. As previously mentioned, X-ray crystallographic analysis of *c*-**C4** revealed that the scrambling side reactions occurred. Observation of the crystal structures of **C2**, **C3**, ***t*-C4**, ***c*-C4**, and **P3** showed that the dihedral angles between of the adjacent pyrrole rings in the spiroadamantyl-substituted *meso*-positions were narrower than in the dimethyl-substituted or unsubstituted *meso*-positions probably due to steric hindrance. This idea is also supported by the fact that our previous examples with spirofluorenyl substituents exhibited wider dihedral angles than the currently and previously discussed dialkyl derivatives.[1,2]



REFERENCES

1. Suzuki M, Suzuki Y and Uetake Y. *J. Porphyr. Phthalocyanines* 2023; **27**: 1097–1102.
2. Suzuki M and Tsurumi, E. Y. *J. Porphyr. Phthalocyanines* 2025; **29**: 280–286.

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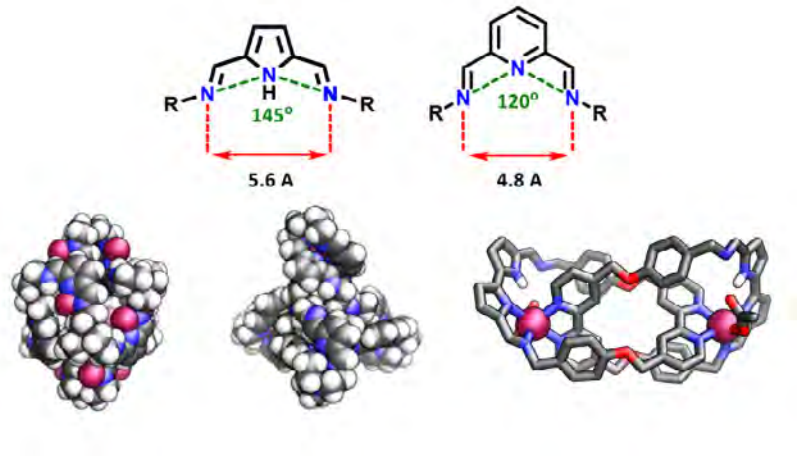
Tautomerism and Dynamics – Two Sides of the Same Coin. Metallosupramolecular Assemblies Based on Iminopyrroles

Bartosz Szyszko[a]

[a]*Faculty of Chemistry, University of Wroclaw, 14 F. Joliot-Curie St., 50-383 Wroclaw, Poland*

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Subcomponent self-assembly is a powerful synthetic tool that enables the construction of remarkably complex metallosupramolecular architectures from relatively simple building blocks.[1] One of the most commonly used motifs in supramolecular chemistry is iminopyridine, owing to its excellent coordination properties. For several years, our group has been exploring metallosupramolecular systems built on the iminopyrrole motif. Using this approach, we have obtained a range of systems, including macrocycles [2,3] as well as cages [4-6] and molecular knots and links [7,8]. At the same time, we have demonstrated that these systems exhibit intriguing properties and reactivity, namely iminopyrrole–aminoazafullvene tautomerism[6] and dynamic behavior,[2,7,8] which govern the behavior of our systems in solution and, in some cases, determine the formation of a specific architecture in the presence of a template.



REFERENCES

[1] Nitschke, J. R. *Acc. Chem. Res.* **2007**, *40*, 103–112.
[2] Matviyishyn, M.; Białońska, A.; Szyszko, B. *Angew. Chem. Int. Ed.* **2022**, *61*, e202211671.
[3] Matviyishyn, M.; Konieczny, K. A.; Trzaskowski, B.; Szyszko, B. *Chem. Eur. J.* **2024**, e202402932.
[4] Sarwa, A.; Białońska, A.; Garbicz, M.; Szyszko, B. *Chem. Eur. J.* **2023**, chem.202203850.
[5] Trzaskowski, B.; Martínez, J. P.; Sarwa, A.; Szyszko, B.; Goddard, W. A., III. *J. Phys. Chem. A* **2024**, *128*, 3339–3350.
[6] Sukiennik, J.; Sarwa, A.; Perdek, J. P.; Siczek, M.; Szyszko, B. *Chem. Eur. J.* **2025**, e202502714.
[7] Sarwa, A.; Białońska, A.; Sobieraj, M.; Martínez, J. P.; Trzaskowski, B.; Szyszko, B. *Angew. Chem. Int. Ed.* **2024**, *63*, e202316489.
[8] Sarwa, A.; Matviyishyn, M.; Perdek, J. P. ; Trzaskowski, B. ; Kulesza, D. ; Zych, E. ; Szyszko, B. *Chem. Commun.* **2026**, *62*, 148–151.

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CD47 peptide-albumin cloaked mesoporous silica nanoparticles for enhanced macrophage evasion and synergistic chemo-photodynamic therapy

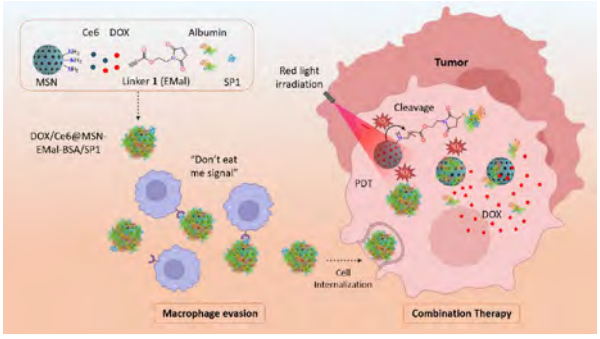
Pontón, I., Núñez, S., Díaz-Perlas, C., Oller-Salvia, B., Semino, C., Sánchez-García, D.

Institut Químic de Sarrià, Universitat Ramon Llull, Via Augusta, 390, Barcelona 08017, Spain.

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Our group has been focusing on the development of drug delivery systems (DDSs) for the controlled delivery of chemotherapeutics and photosensitizers [1]. A key feature of a efficient DDS is its ability to selectively accumulate in tumor tissues. To achieve this, DDSs must circulate in the bloodstream long enough to increase their chances of tumor accumulation. Nevertheless, once injected into the blood, nanoparticles (NPs) quickly become covered by plasma proteins, creating a protein corona (PC) in seconds. The binding of certain native proteins, known as opsonins, triggers the removal of up to 95 % of injected NPs by the mononuclear phagocyte system.

In this study [2], we developed a nanocarrier based on mesoporous silica nanoparticles coated with a light-responsive PC that prevents macrophage recognition and enables the controlled release of doxorubicin (DOX). The PC consists of bovine serum albumin anchored to the NP surface through a novel singlet oxygen-sensitive linker, with further functionalization using a CD47-mimetic peptide (SP1) to enhance immune evasion. BSA coating resulted in a 1.9-fold reduction in uptake by macrophage cultures compared to uncoated MSNs. Incorporation of SP1 further diminished macrophage internalization by 3.5-fold, as quantified by *in vitro* assays. Irradiation with red light (660 nm) triggers cleavage of the singlet oxygen-sensitive linker, leading to PC shedding and subsequent DOX release. *In vitro* cytotoxicity evaluations against pancreatic cancer cell lines demonstrated potent efficacy. This high cytotoxicity is attributed to a synergistic effect resulting from the photodynamic generation of singlet oxygen by chlorin e6 (Ce6) and the chemotherapeutic action of the released DOX.



REFERENCES

1. Martínez-Edo, G.; Xue, E.Y.; Ha, S.S.Y.; Pontón, I.; González-Delgado, J.A.; Borrós, S.; Torres, T.; Ng, D.K.P.; Sánchez-García, D. *Chem. Eur. J.* **2021**, *27*, 14610–14618.
2. Pontón, I.; Núñez, S.; Díaz-Perlas, C.; Oller-Salvia, B.; Semino, C.; Sánchez-García, D. *J. Drug Deliv. Sci. Technol.* **2026**, *115*, 107851.

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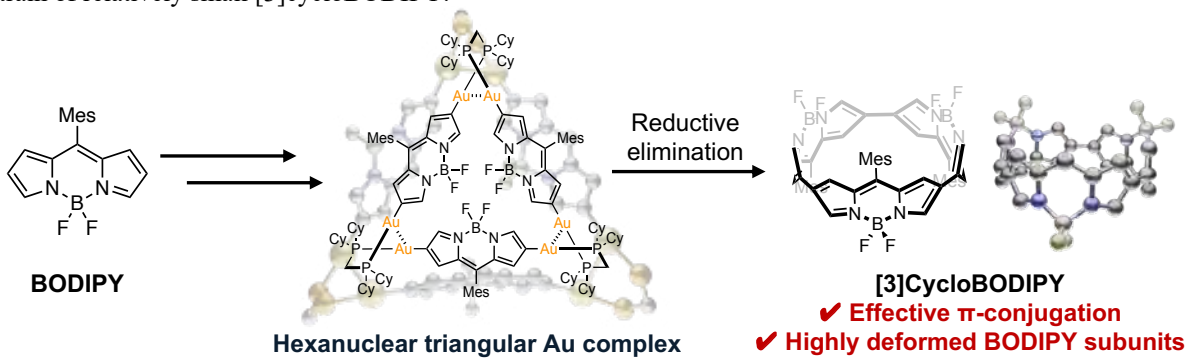
Synthesis and Properties of [3]CycloBODIPY: A Highly Strained Pyrrole-Based Macrocyclic π-System

Hideaki Takano[a,b], Masaki Sugino[a], Yoshitaka Tsuchido[c], Rento Maeda[d], Ichiro Hisaki[d], Hiroshi Shinokubo[a]

[a]*Department of Molecular and Macromolecular Chemistry, Graduate School of Engineering, Nagoya University, Chikusa-ku, Nagoya, Aichi 464-8603, Japan*
[b]*Institute for Advanced Research, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, Aichi 464-8601, Japan*
[c]*Department of Chemistry, Faculty of Science, Tokyo University of Science, Shinjuku-ku, Tokyo 162-8601, Japan*
[d]*Division of Chemistry, Graduate School of Engineering Science, The University of Osaka, 1–3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan*

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Boron dipyrromethenes (BODIPYs) have fascinating photophysical properties, including intense visible-light absorption and emission with high quantum yields.[1] Macrocyclic compounds containing BODIPY subunits have been extensively investigated to date due to their diverse application in sensing, lasing, and photodynamic therapy.[2] However, the macrocyclic compounds composed only of BODIPY subunits remain elusive. Herein, we have achieved the synthesis of the macrocyclic BODIPY trimer, namely [3]cycloBODIPY, through the reductive elimination from the hexanuclear triangular Au complex.[3] [3]CycloBODIPY shows NIR absorption originating from effective π-conjugation between BODIPY subunits and deformation of the BODIPY π-skeleton. Furthermore, we have elucidated that the flexibility of sp^3 boron centers on BODIPY subunits relieves the ring strain of relatively small [3]cycloBODIPY.



REFERENCES

1. (a) Loudet, A.; Burgess, K. *Chem. Rev*. **2007**, *107*, 4891–4932. (b) Boens, N.; Verbelen, B.; Ortiz, M. J.; Jiao, L.; Dehaen, W. *Coord. Chem. Rev.* **2019**, *399*, 213024.
2. Qin, Y.; Liu, X.; Jia, P.-P.; Xu, L.; Yang. H.-B. *Chem. Soc. Rev*. **2020**, *49*, 5678–5703.
3. Sugino, M.; Tsuchido, Y.; Maeda, R.; Hisaki, I.; Takano, H.; Shinokubo, H. *Angew. Chem. Int. Ed*. **2025**, *64*, e202519612.

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Oligoglucosamine as a Biomass-Derived Aqueous Platform for Metalloporphyrin Photosensitizers

Yuta Takano[a,b], Kushal Mohan Gowda[b], Yasuko Osakada[c,d], Mamoru Fujitsuka[c,d], Vasudevanpillai Biju[a,b]

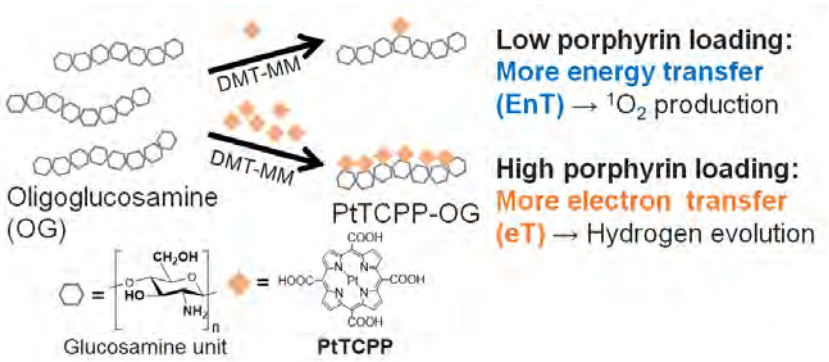
[a] *Research Institute of Electronic Science, Hokkaido University, Sapporo, Japan*
[b] *Graduate School of Environmental Science, Hokkaido University, Sapporo, Japan*
[c] *SANKEN (The Institute of Scientific and Industrial Research), The University of Osaka, Ibaraki, Japan*
[d] *Open and Transdisciplinary Research Initiatives (ICS-OTRI), The University of Osaka, Suita, Japan*

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Metalloporphyrins are versatile photosensitizers applicable to photodynamic therapy (PDT) and photocatalytic energy conversion. The use of water as a reaction medium is essential for biomedical applications such as PDT and for the development of sustainable photocatalytic systems. However, metalloporphyrins are prone to intermolecular π-π stacking aggregation in aqueous environments, which often perturbs their excited states and diminishes photosensitizing efficiency. Here, we report that oligoglucosamine (OG; average degree of polymerization ≈ 7) serves as an effective aqueous platform for metalloporphyrins. OG is a biomass-derived sustainable material whose suitability as a porphyrin platform arises from its multiple free amino groups available for covalent conjugation and intrinsic amphiphilicity. [1] Moreover, we demonstrate that OG enables switching of intermolecular electronic interactions between porphyrin moieties (**Scheme**).

Covalent PtTCPP-OG conjugates were synthesized at various loading ratios (0.10-1.0 eq per glucosamine unit) of platinum porphyrin (PtTCPP) using DMT-MM as an amide coupling reagent. The conjugates exhibited loading-dependent changes in UV-vis absorption, phosphorescence intensity, and hydrodynamic diameter by DLS. Singlet oxygen ($^1O_2$) generation efficiency decreased with increasing PtTCPP content, consistent with triplet-state self-quenching at higher loadings. Methylene blue photodegradation was observed for all conjugates; notably, the product distribution implied a mechanistic shift from an energy transfer pathway ($^1O_2$-mediated oxidation) to an electron transfer-dominant pathway at higher PtTCPP loadings, which was further supported by time-resolved transient absorption spectroscopy.

As a proof-of-concept for the electron transfer pathway, photocatalytic hydrogen evolution under blue LED irradiation (405 nm, 400 mW cm^{-2}) with ascorbic acid as a sacrificial reductant afforded substantial H_2 production (≥ 80 mmol g^{-1} h^{-1}). These findings establish PtTCPP-OG as a tunable photosensitizing platform applicable to both oxidative (PDT-type) and reductive (solar fuel generation) photochemical transformations.



Scheme. Loading-dependent switching of photoreactivity in PtTCPP–OG conjugates.

REFERENCES

1. Askari, S. et al. *Carbohydr. Polym.*, **2026,** *371*, 124522.

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π-Dimer of an Antiaromatic HomoHPHAC Monocation

Masayoshi Takase

Graduate School of Science and Engineering, Ehime University, Matsuyama 790-8577, Japan

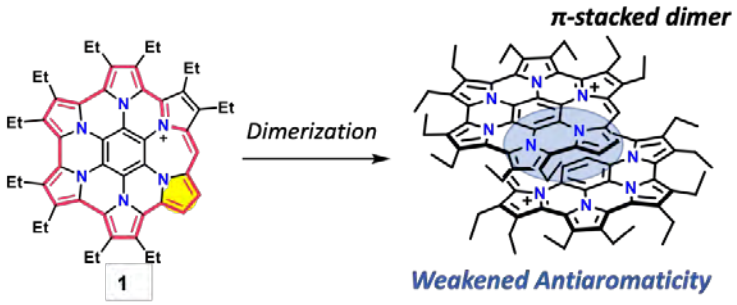
Antiaromatic π-conjugated molecules are inherently destabilized by cyclic electron delocalization and therefore rarely exhibit well-defined intermolecular aggregation. Nevertheless, theoretical studies have suggested that π-stacking of antiaromatic systems can alleviate their intrinsic antiaromaticity through intermolecular orbital interactions. Experimental demonstrations of such behavior, particularly for closed-shell charged molecules, remain limited.

Herein, I report the synthesis and aggregation behavior of a sterically unencumbered antiaromatic homoHPHAC monocation that lacks substituents at the *meso* position and adjacent pyrrolic *β* positions [1]. This molecular design enables close intermolecular contact at the π surface. Single-crystal X-ray diffraction analysis revealed that **1** adopts a highly planar conformation and unexpectedly forms a slipped π-stacked dimer in the solid state, despite its monocationic nature. The intermolecular separation within the dimer is comparable to that observed in typical π-stacked systems.

Concentration- and temperature-dependent ^{1}H NMR measurements demonstrated that a similar monomer–dimer equilibrium operates in solution. Analysis of the concentration-dependent chemical shift changes afforded an association constant on the order of 10^{2} M^{-1} in acetone-d_6 at room temperature. Variable-temperature studies further indicated that dimer formation is enthalpically favored, consistent with stabilization driven by π–π interactions.

Structural and computational analyses suggest that aggregation leads to partial alleviation of the intrinsic antiaromaticity of the homoHPHAC core. Bond-length-based aromaticity indices show increased delocalization upon dimer formation, while anisotropy of the induced current density calculations reveal a reduced paratropic ring current in the dimer relative to the monomer [2]. DFT calculations further indicate that intermolecular orbital interactions stabilize the dimer through the formation of quasi-degenerate frontier orbitals.

In this presentation, I will discuss the synthesis of the newly developed homoHPHAC, its π-dimer formation in solution and in the solid state, and the accompanying changes in antiaromaticity.



REFERENCES

1. Wada, K. et al., *submitted for publication*.
2. Oki, K. et al., *J. Am. Chem. Soc.* **2019**, *141*, 16255.

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Asymmetrically coordinated chlorophylls in natural and artificial systems

Hitoshi Tamiaki and Shin Ogasawara

Graduate School of Life Sciences, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan

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Chlorophyll (Chl) *a* (Fig. 1, left) is one of the most important porphyrinoid pigments in oxygenic phototrophs [1]. Since the central Mg atom in its cyclic tetrapyrrole (chlorin) is highly coordinatable, all the Chl-*a* molecules are axially bound with a single ligand in photosynthetically active apparatuses to give its five-coordinated (5-C) species. The axial coordination makes asymmetry around the central Mg atom due to the regio-differently situated peripheral substituents. X-ray crystallographic and cryo-electron microscopic analyses reveal that α-ligations are preferable over β-ligations in the natural Chl–peptide complexes [2]. To mimic the 5-C Chl-*a* epimers, we here report asymmetrically axial-ligated trivalent metal complexes of a Chl-*a* derivative in a solution [3].

Methyl pyropheophorbide *a*, one of the Chl-*a* derivatives, was reacted with Ga/In/Tl(III)X_3 to give the corresponding M(III) complexes **1** with a single anionic L ligand. Their ^{1}H NMR spectra in $CDCl_3$ indicated that the synthetic M(III) chlorins with an axial ligand were epimeric mixtures **1**-α/β around the central metal (Fig. 1, center/right). Molecular model calculation proposed their absolute configurations at the central M(III) atom. The α-ligated complexes **1**-α were estimated to be favorable over the β-ligated epimers **1**-β. The observed epimeric ratios varying 1.3 to 2.0 were dependent on the central metals M and axial ligands L. The preferable production of the α-epimers in these group-13 metal complexes is consistent with the predominantly α-ligated Mg(II) complexes in photosynthetic Chl–peptides. The diastereomeric discrimination of the synthetic models in a solution at room temperature due to the tight ionic coordination is in sharp contrast to that such epimers could not be visible for any divalent metal [Mg/Zn(II)] complexes in solution-based NMR measurements because of the rapid ligand exchange.

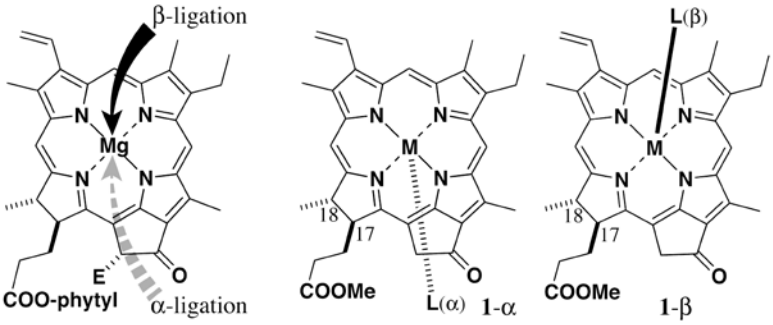


Fig. 1. Molecular structures of naturally occurring Chl *a* with axial ligation sites (E = COOMe, left) and synthetic metal (M) complexes of methyl pyropheophorbide *a* as a Chl-*a* derivative axially α/β-ligated with a single ligand L (**1**-α/β, center/right).

REFERENCES

1. H. Tamiaki, S. Kichishima, *Plant Cell Physiol*., **66**, 153–167 (2025).
2. H. Tamiaki, *Fundamentals of Porphyrin Chemistry: A 21st Century Approach*, vol. 2, ch. 17, John Wiley & Sons, West Sussex, UK, 2022; 743–776. doi: 10.1002/9781119129301.ch17
3. S. Ogasawara, H. Ishikawa, Y. Kinoshita, H. Tamiaki, *J. Phys. Org. Chem.*, **39**, e70046 (2026).

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Electrolytic Synthesis of Porphyrinic Zr Metal-Organic Frameworks with Selective Crystal Topologies

Daisuke Tanaka[a]

[a]*Department of Chemistry, School of Science, Kwansei Gakuin University*

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Recently, the electrochemical synthesis of metal–organic frameworks (MOFs) has gained significant attention as a potential industrial technique because it enables the direct in situ growth of MOFs on conductive substrates. Both anodic dissolution and cathodic deposition strategies have been explored to construct diverse MOF architectures. Among them, zirconium(IV)-based MOFs have been extensively studied owing to their remarkable chemical and thermal robustness. Nevertheless, the electrochemical preparation of Zr-MOFs remains challenging, as the zirconium-based clusters are highly sensitive to subtle variations in reaction parameters, including concentration, temperature, and reaction time. The introduction of carboxylic acid modulators has proven particularly effective in directing cluster formation. Furthermore, the ability to regulate polymorphism and defect structures in Zr-MOFs represents a major focus in this field. Electrochemical processes typically proceed as interfacial heterogeneous reactions near the electrodes, where the distribution of reactants differs from that in conventional homogeneous systems. Because the precursor species are concentrated locally at the electrode surface, the chemical reactivity in electrolysis differs from that in bulk solution reactions. Thus, strategies for controlling MOF topologies during electrochemical synthesis have not yet been fully clarified.

Herein, we report the anodic dissolution synthesis of porphyrinic Zr-MOFs, yielding both the thermodynamically stable (PCN-222) and kinetically favored (PCN-224) phases.[1] To the best of our knowledge, this work constitutes the first example in which MOF polymorphism has been successfully tuned by electrolysis. The selective crystallization of PCN-222 was found to require the transient formation of an amorphous phase on the electrode at the initial stage. These results demonstrate that interfacial reaction dynamics—and consequently the resulting MOF topologies—can be effectively controlled by adjusting electrochemical parameters. This study offers new insights toward establishing a precise electrolytic route for MOF synthesis.

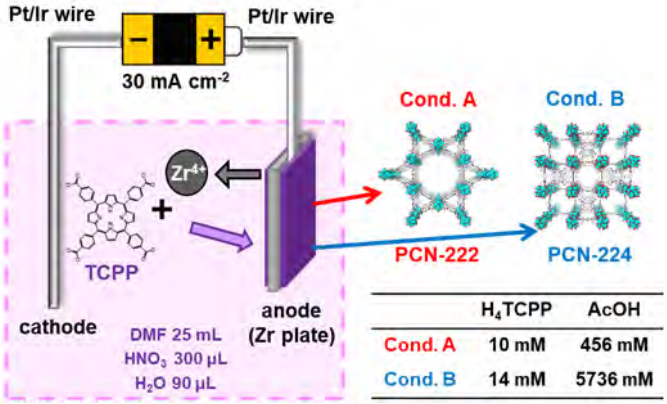


Figure 1. Synthesis scheme of Porphyrinic Zr Metal-Organic Frameworks and the reaction conditions.

REFERENCES

1. K. Okada, Y. Tanaka, T. Inose, H. Uji-i, H. Yoshikawa, D. Tanaka*, *Dalton Trans.* **2021**, *50*, 5411-5415.

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Aza[n]circulenes: Novel Pyrrole-fused Polycycles

Takayuki Tanaka[a], **Yoh Kumagai**[a], **Yusuke Matsuo**[a], **Shu Seki**[a]

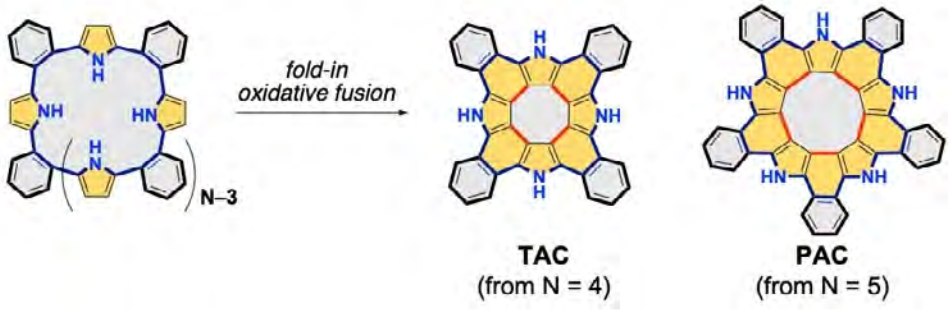
[a]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Japan*

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Hetero[n]circulenes are polycyclic heteroaromatic molecules that have a central n-membered ring surrounded by n-sided benzene and heteroaromatic segments. While the first report on tetraoxa[8]circulene dates back to 1968, new hetero[n]circulene derivatives containing units other than furan had not been explored until the report on azatrioxa[8]circulene in 2013. Still, all-aza hetero[8]circulenes had not been reported until our first report on tetraaza[8]circulene in 2015.[1] Aza[8]circulenes were expected to be attractive functional molecules because of their electron-rich properties and possible N-substitutions. In addition, the (anti)aromaticity of their cyclooctatetraene-type segments was a topic of interest both experimentally and theoretically.

To address novel aza[n]circulene systems, we have explored a new synthetic protocol, so-called "*fold-in*" synthesis. Firstly, *ortho*-phenylene-bridged cyclic oligopyrroles were prepared by coupling reactions.[2–4] These cyclic oligopyrroles can be regarded as porphyrin(2.2.2.2) for N = 4, and pentaphyrin(2.2.2.2.2) for N = 5, although they do not exhibit global macrocyclic aromaticity due to the localized aromaticity on pyrrole and benzene segments as well as their highly twisted structures observed in the solid state. Then, the cyclic precursors were subjected to oxidation conditions to connect neighboring pyrrole units with inside-out flipping. These "*fold-in*" reactions successfully afforded tetraaza[8]circulene (**TAC**) from tetrapyrrole and pentaaza[10]circulene (**PAC**) from pentapyrrole in moderate to good yields.

X-Ray diffraction analysis revealed the planar structure of **TAC**. The C–C bond lengths of the central eight-membered-ring are in the range of 1.43-1.44 Å. Consistent with the Clar's sextet rule, this molecule can be regarded as a polycyclic aromatic molecule and the 8π antiaromatic resonance contribution is considered to be negligible. The structure of **PAC** was revealed to be saddle-distorted and the bond lengths of the central ten-membered-ring are in the range of 1.45-1.49 Å, again indicating the negligible contribution of 10π aromaticity in the central decagon. The conformation is quite flexible in solution as the estimated saddle-to-saddle inversion barrier is 3.0 kcal/mol. These novel aza[n]circulenes are soluble in THF and DMSO despite the absence of sterically hindered substituents due to hydrogen bonding at the NH site with solvent molecules. Both **TAC** and **PAC** exhibit well-structured absorption and emission spectra in the visible region.



REFERENCES

1. F. Chen, Y. S. Hong, S. Shimizu, D. Kim, T. Tanaka, A. Osuka, *Angew. Chem. Int. Ed.* **2015**, *54*, 10639.
2. Y. Morimoto, F. Chen, Y. Matsuo, K. Kise, T. Tanaka, A. Osuka, *Chem. Asian J.* **2021**, *16*, 648.
3. Y. Morimoto, A. Osuka, T. Tanaka, *J. Porphyrins Phthalocyanines* **2021**, *25*, 937.
4. Y. Matsuo, K. Kise, Y. Morimoto, A. Osuka, T. Tanaka, *Angew. Chem. Int. Ed.* **2022**, *61*, e202116789.

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Spin Selective Catalysis with Chiral Metal-Organic Frameworks

Francesco Tassinari[a], Martina Campi[b], Valeria Iacomini[b], Roberto Biagi[b], Andrea Cornia[a], Alessio Nicolini[a]

[a]University of Modena and Reggio Emilia, Department of Chemical and Geological Sciences, Via G. Campi 103, 41125, Modena (MO), Italy; [b]University of Modena and Reggio Emilia, Department of Physical, Computer and Mathematical Sciences, Via G. Campi 213/a, 41125, Modena (MO), Italy

The regulation of the electron spin states at the active sites of catalysts can be an effective strategy to modify the reaction pathway or to reduce the activation energy required for spin-dependent reactions [1]. This spin-engineered catalysis can thus grant improved catalytic efficiency and selectivity for certain reactions of importance for sustainable chemistry, such as the Oxygen Evolution Reaction (OER) or CO_2 fixation [2-4]. There are different strategies that can afford control over the spin states in catalysts and that don't rely on the simple application of an external magnetic field; in our studies we use chirality as the tool that allows control over the electron spin, exploiting the Chirality-Induced Spin Selectivity (CISS) effect [5], which couples the electron linear momentum with its spin. In particular, our approach consists in exploiting chiral Metal-Organic Frameworks (χ-MOFs) as the catalysts of choice, since they have well-defined structures and properties that are tunable through chemical design, allowing to study in detail the structure-properties relationship.
In this contibution, we present few examples of different χ-MOFs we synthetised and characterized over the last few months and their applications as catalysts for important sustainable energy conversion technologies.

REFERENCES

[1] Zhang, B. et al., *Chem. Soc. Rev.* **2025**, 54 (22), 10616–10653.
[2] Dai, J. et al., *Nat Commun* **2024**, 15 (1), 88.
[3] Mtangi, W.et al., *JACS* **2017**, 139 (7), 2794–2798.
[4] Fang, Y. et al., *Chem* **2023**, 9 (2), 460–471.
[5] Bloom, B. et al., *Chem. Rev.* **2024**, 124 (4), 1950–1991.

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Rhodium Porphyrin-Based Catalysts for Ammonia Borane Hydrolytic Dehydrogenation

Francesca Tessore[a], **Ilaria Barlocco**[a], **Gabriele Di Carlo**[a], **Manuel Minnucci**[a], **Elisa Pianta**[a], **Alberto Villa**[a]

[a]*Department of Chemistry, University of Milan, via Golgi 19 20133 Milan (Italy)*

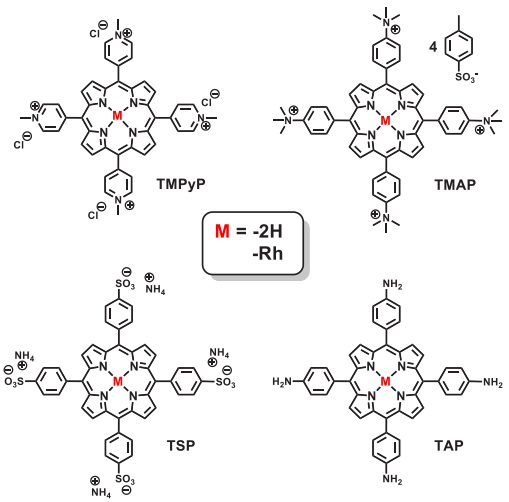
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The transition from fossil fuels to sustainable energy sources has intensified interest in hydrogen as a clean energy carrier. Ammonia borane (AB) is a promising hydrogen storage material due to its high gravimetric hydrogen capacity and stability; however, its thermal decomposition requires high temperatures and produces undesired byproducts. In contrast, catalytic hydrolysis of AB in water enables efficient hydrogen release under mild conditions according to:

$$NH_3BH_3 + 2H_2O \rightarrow NH_4^+ + BO_2^- + 3H_{2(g)}$$

Rhodium-based catalysts are among the most effective for AB hydrolysis at room temperature [1]. Porphyrins, featuring a rigid aromatic framework and an inwardly oriented N_4 coordination pocket, offer a well-defined environment for stabilizing rhodium centers. To date, rhodium–porphyrin systems have been limited to nanoparticle-stabilized composites, while single-site molecular catalysts remain largely unexplored.

Herein, we report the first rhodium porphyrins operating as single-site catalysts for the hydrolytic dehydrogenation of AB in aqueous media under mild conditions. Rhodium complexes were synthesized from $RhCl_3 \cdot 3H_2O$ and four free-base porphyrins, including water-soluble cationic and anionic ligands for homogeneous catalysis and a neutral, insoluble porphyrin for heterogeneous catalysis.



All catalysts were fully characterized by spectroscopic techniques and ICP-OES.

All rhodium porphyrins exhibited catalytic activity at 303 K and 1 atm, with the anionic TSP_Rh showing the highest performance. While ionic, water-soluble catalysts experienced gradual deactivation, the heterogeneous TAP_Rh catalyst remained stable over multiple cycles, albeit with lower activity [2]. These findings demonstrate the viability of rhodium porphyrins as efficient homogeneous and heterogeneous catalysts for ultra-pure hydrogen generation from AB and motivate further development of rhodium porphyrin-based covalent organic frameworks for enhanced catalytic performance.

REFERENCES

1. Akbayrak, S. ; Tonbul, Y. ; Özkar, S. *ACS Sustainable Chem. Eng.* **2020**, *8*, 4216.
2. Minnucci, M.; Barlocco, I.; Prati, L. ; Stucchi, M. ; Villa, A. ; Di Carlo, G. Tessore, F. *Dalton Trans.* **2026**, *accepted*.

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Vertically Aligned Chiral Low-Resistance Porphyrin Wires Enable Spin Valves without Ferromagnetic Contacts

Jiaqi Zhu,[a,†] Elizabeth Shiby,[b] Anu Gupta,[c] Brian P. Bloom,[b] Anisha Mondal,[b] Chih-Hung Ko,[a] Victoria L. Cinnater,[a] Jonas Fransson,[d] Yossi Paltiel,[e] Ron Naaman,[c] David H. Waldeck,[b] and Michael J. Therien[a]

[a]*Department of Chemistry, Duke University, Durham, North Carolina 27708, USA*
[b]*Department of Chemistry, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA*
[c]*Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot 7610001, Israel*
[d]*Department of Physics and Astronomy, Uppsala University, Uppsala 75221, Sweden*
[e]*Institute of Applied Physics, Hebrew University of Jerusalem, Jerusalem 91904, Israel*

Switches that turn current on and off in response to external stimuli are the basis of any information transfer or processing system. In common electronics, this function is performed by transistors. In spintronics, where information is encoded in the properties of electrons' spins, this can be achieved either with spin transistors or spin valves. We describe a spin valve system that operates without any ferromagnetic element and is activated by a weak external magnetic field. This system is based on a chiral multi-porphyrin molecular wire that features a terminal Cu(II) spin center and forms vertically aligned self-assembled monolayers (SAMs) on metal substrates. Spin transport and magnetic properties of these SAMs demonstrate not only that the chirality-induced spin selectivity (CISS) effect drives a spin-polarized current in these assemblies: activation of these systems with an external magnetic field gives rise to ambient temperature spin valve behavior, and highlights that these chiral SAMs display thermally activated ferromagnetism.

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Tuning Charge Transfer in Porphyrins for Photocatalysis

Haining Tian[a]

[a]*Physical Chemistry, Uppsala University, Box 523, 75120 Uppsala, Sweden*

Efficient light-harvesting systems with fast photoinduced charge separation and long-lived charge-separated states are essential for solar energy conversion and sustainable photocatalysis, yet remain challenging to realize. Here, we present two complementary porphyrin–viologen-based strategies that address these challenges through controlled molecular assembly. In the first approach, a zinc porphyrin–viologen dyad is covalently linked and self-assembled into nanoparticles in aqueous solution.[1] While no electron transfer is observed in monomeric dyads in organic solvent, nanoparticle formation induces rapid charge separation and affords a remarkably long-lived charge-separated state with a lifetime of up to 4.3 ms, attributed to aggregation-induced electronic interactions and charge hopping. These nanoparticles exhibit significantly enhanced photocatalytic hydrogen evolution compared to porphyrin-only nanoparticles. In the second approach, an electrostatically assembled porphyrin–viologen system serves as a stable, recyclable heterogeneous photocatalyst for selective organic oxidation.[2] Efficient charge separation between a sulfonated porphyrin donor and benzyl viologen acceptor promotes superoxide generation, enabling quantitative and highly selective oxidation of aryl sulfides to sulfoxides under mild conditions, with excellent catalyst recyclability. Together, these results demonstrate how molecular and supramolecular design of porphyrin–viologen assemblies can dramatically extend charge-separated state lifetimes and unlock efficient photocatalytic transformations relevant to solar fuel production and green organic synthesis.

REFERENCES

1. B. Cai, H. Song, A. Brnovic, M. V. Pavliuk, L. Hammarström, H. Tian, *J. Am. Chem. Soc.* **2023** *145* (34), 18687-18692.
2. B. Cai, P. Huang, Y. Fang, H. Tian, *Adv. Sci.* 2024, 11, 2308469.

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Electrocatalysis of Heme Enzymes, Beyond Substrate Sensing / Degradation

Smilja Todorovic[a], Célia M. Silveira[a], Angelique Pothuizen[b], Marc J. F. Strampraad[b], Frank Hollmann[b] and Peter-Leon Hagedoorn[b]

[a]*Instituto de Tecnologia Química e Biológica António Xavier, Universidade NOVA de Lisboa, Av. da República, 2780-157 Oeiras*
[b]*Department of Biotechnology, Delft University of Technology, Delft, The Netherlands*

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Understanding how the protein environment governs the chemistry of the heme and how to translate these intrinsic traits into efficient bioelectronic devices paves the way for exploiting these exceptionally diverse biocatalysts for biotechnological applications. Heme enzymes offer unmatched alternatives for driving thermodynamically unfavorable chemical reactions, where synthetic catalysts perform poorly. In parallel, they provide superior capacity to sensitively and selectively detect small molecules that are their (co)substrates.

Here, we demonstrate how understanding the structural and thermodynamic properties of dye decolorizing peroxidases (DyPs), chlorite dismutases (Clds), and unspecific peroxygenases (UPOs) in solution can guide their application in the development of 3rd-generation bioelectronic devices that rely on immobilized enzymes. These heme b-containing enzymes all catalyze ´difficult´ chemical reactions, including i) the oxidation of chemically inert and environmentally harmful synthetic dyes and phenolic and nonphenolic lignin units with concomitant reduction of hydrogen peroxide (DyPs) [1], ii) the decomposition of chlorite to harmless chloride that occurs via the rare enzymatic formation of O-O bond (Clds) [2], and iii) the selective peroxide-dependent monooxygenation of versatile substrates, which is among the most essential reactions in organic synthesis (UPOs) [3]. For these reasons, these enzymes have attracted significant biotechnological interest; however, their actual applications have lagged behind. We show here a comparative study of DyP, Cld and UPO, using resonance Raman spectroscopy (RR) and electrochemistry to reveal fine details about the active site structure and thermodynamic properties of these enzymes in solution, and surface enhanced RR (SERRS) spectroelectrochemistry to disclose their structural and (electro)catalytic properties in the immobilized state [1]. Some of the studied enzymes represent excellent candidates, exhibiting activity and efficient redox chemistry upon attachment to electrode interfaces, which will allow us to advance their biotechnological applications, while others still face challenges despite their unique structural and catalytic properties in solution.

REFERENCES

1. C. Barbosa, M. C. Stefoni, C. F. Rodrigues, L. O. Martins, D. H. Murgida, S. Todorovic, and C. M. Silveira ACS Omega 2025 10 8736-8744
2. J. Püschmann, D. Mahor, D. C. de Geus, M. J. F. Strampraad, B. Srour, W. R. Hagen, S. Todorovic, and P.-L. Hagedoorn, ACS Catalysis 2021 11 14533-14544
3. F. Tonin, F. Tieves, S. Willot, A.Van Troost, R. Van Oosten, S. Breestraat, S. Van Pelt, M. Alcalde, and F. Hollmann, Organic Process Research and Development 2021, 25 1414-1418

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Molecular mechanisms of heme-based oxygen sensor protein in bacterial chemotaxis

Rei Tohda[a], Yukino Tsuji[a], Norifumi Muraki[b], Seiki Baba[c], Hideo Okumura[c], Yoshiaki Kawano[d], Takeshi Yokoyama[e], Takehiko Tosha[a], Shigetoshi Aono[f]

[a] *Graduate School of Science, University of Hyogo, Japan,*
[b] *Bioresources Engineering Research Institute, Ishikawa Prefectural University, Japan,*
[c] *Structural Biology Division, Japan Synchrotron Radiation Research Institute, Japan,*
[d] *Advanced Photon Technology Division, RIKEN SPring-8 Center, Sayo-gun, Hyogo, Japan,*
[e] *Graduate School of Life Sciences, Tohoku University, Japan,*
[f] *Institute for Molecular Science, National Institutes of Natural Sciences, Japan*

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Gas molecules, including dioxygen (O_2) and nitric oxide, are known to function as "signal molecules" that regulate various physiological processes such as chemotaxis, gene expression, and metabolic control via second messenger synthesis. In these systems, signal transduction proteins that selectively recognize gas molecules detect external signals to regulate physiological processes. O_2 plays a critical role as a signal molecule in bacterial chemotaxis, so-called aerotaxis—the directed movement of bacteria toward optimal oxygen concentrations. This behavior is controlled by HemAT (Heme Aerotaxis Transducer protein), a heme-based sensor protein [1]. HemAT consists of two functional domains, the sensor domain and the signaling domain. The N-terminal sensor domain has structural similarity to myoglobin and binds oxygen using its heme. The C-terminal signaling domain is homologous to MCPs (methyl-accepting chemotaxis proteins) and transmits signals to Che proteins (histidine kinase CheA, adaptor protein CheW, and response regulator CheY). It is thought that HemAT forms a complex with CheA and CheW proteins to control bacterial flagellar rotation in aerotaxis. Despite its importance, the molecular mechanisms of oxygen sensing and signal transduction are poorly understood.

To understand the sensing and signaling mechanisms in the HemAT system, we aimed to determine the structures of O_2-bound and deoxy forms of HemAT and its complex with Che proteins by X-ray crystallography and cryo-electron microscopy (cryo-EM).

We determined the crystal structures of the O_2-bound and deoxy forms of the HemAT sensor domain at 2.36 Å resolution. Comparison of these structures revealed dynamic changes in the proximal region of HemAT upon O_2 binding. In the oxygen-bound form, a hydrogen bonding network was formed in the proximal region, which stabilizes the structure of the helix connecting to the signaling domain. In contrast, this helix region was disordered due to the absence of the hydrogen bonding network in the deoxy form. These findings suggest that O_2 binding at the heme distal site induces conformational changes at the heme proximal site that possibly works as a part of signal transduction to the signaling domain through the changes in the structural stability of the linker region between the sensor and the signaling domains in HemAT. To further understand the signaling mechanism in the HemAT system, we also performed cryo-EM measurement to determine the structure of full-length HemAT and its complex with CheA/CheW, and carried out in vitro phosphorylation assays. Preliminary analysis has revealed the structure of full-length HemAT at 4.77 Å resolution, and confirmed that the HemAT/CheA/CheW complex phosphorylates CheY. In this presentation, we will discuss the molecular mechanisms of oxygen sensing and signal transduction based on these structural findings.

REFERENCES

1. Hou, S. *et. al*., Myoglobin-like Aerotaxis Transducers in Archaea and Bacteria, *Nature*, 2000, 403 (6769), 540–544.

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Tripyrrindione Radicals: Metal Coordination, Redox Chemistry, and anti-Kasha Fluorescence

Elisa Tomat[a,b], Iva Habensus,[b] Lily J. North,[b] Clayton J.Curtis,[b] Andrei V. Astashkin[b]

[a] *University of Vienna, Institute of Inorganic Chemistry, Faculty of Chemistry, Währinger Straße 42, 1090 Wien, Austria. Email: elisa.tomat@univie.ac.at*
[b] *University of Arizona, Dept. of Chemistry and Biochemistry, 1306 E. University Blvd., Tucson, AZ 85721, USA*

Naturally occurring biopyrrin pigments are heme metabolites featuring a conjugated tripyrrolic scaffold and characteristic pyrrolin-2-one termini [1, 2]. Whereas linear tetrapyrroles, such as biliverdin, enforce a helical geometry in metal complexes, the dipyrrin-1,9-dione and tripyrrin-1,14-dione fragments coordinate metals as planar chelates and allow access to the metal center for additional ligands. Critically, these scaffolds serve as robust electron reservoirs via reversible ligand-based redox processes and avoid the irreversible degradation that characterizes other linear oligopyrroles [3, 4]. The tripyrrindione framework has emerged as a versatile coordination platform for multiple transition metals in different oxidation states. We found that several complexes of tripyrrindione radicals are air-stable at room temperature and undergo reversible one-electron processes to access different redox states of the ligand system [3, 5]. Through spectroscopic (EPR, optical absorption) and computational studies, we demonstrated that multi-center interactions between delocalized spins lead to dimers of tripyrrindione radicals in the solid state and at low temperature in solution [6, 7]. Recent reactivity studies indicate that the metal-based reduction of Au(III) tripyrrindione leads to a highly reactive species that utilizes dichloromethane in the formation of a cyclometalated organo-Au(III) complex [8]. Furthermore, our spectroscopic and computational investigations document anti-Kasha fluorescence emission of tripyrrindione radicals bound to closed-shell transition metals (e.g., Zn(II), Ag(I)) [9]. Overall, the portfolio of properties of the redox-active tripyrrindione platform is positioned to offer new opportunities in catalysis, medicinal chemistry, and molecular materials.

REFERENCES

1. Tomat, E., Curtis, C. J. *Acc. Chem. Res.* **2021**, *54*, 4584.
2. Tomat, E. *J. Porphyrins Phthalocyanines* **2019**, *23*, 1265.
3. Gautam, R.; Loughrey, J. J.; Astashkin, A. V.; Shearer, J.; Tomat, *Angew. Chem. Int. Ed.* **2015**, *54,* 14894.
4. Curtis, C. J.; Astashkin, A. V.; Conradie, J.; Ghosh, A.; Tomat, E. *Inorg. Chem.* **2021**, *60*, 12457.
5. Curtis, C. J.; Tomat, E. *J. Porphyrins Phthalocyanines* **2020**, *24*, 112.
6. Gautam, R.; Astashkin, A. V.; Chang, T. M.; Shearer, J.; Tomat, E. *Inorg. Chem.* **2017**, *56*, 6755.
7. Tomat, E.; Curtis, C. J.; Astashkin, A. V.; Conradie, J.; Ghosh, A. *Dalton Trans.* **2023**, *52,* 6559.
8. Curtis, C. J.; Habenšus, I.; Conradie, J.; Bardin, A. A.; Nannenga, B. L.; Ghosh, A.; Tomat, E. *Inorg. Chem.* **2024**, *63,* 17188.
9. Gautam, R.; Petritis, S. J.; Astashkin, A. V.; Tomat, E. *Inorg. Chem.* **2018***, 57,* 15240.

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meso-Edited Phthalocyanine Derivatives

Naoyuki Toriumi[a], **Masanobu Uchiyama**[a]

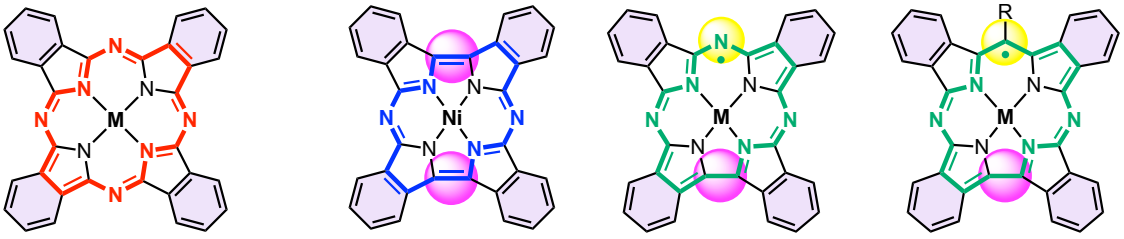
[a]*The University of Tokyo, Graduate School of Pharmaceutical Sciences*

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Porphyrinoids represent a prominent class of π-conjugated aromatic/antiaromatic compounds that are of synthetic, theoretical, and practical interest. Among them, phthalocyanines, composed of four isoindoline units with bridging *meso*-nitrogen atoms, exhibit remarkable physicochemical properties, such as intense absorption/emission in the visible-near-IR region and high electron-accepting ability, and have been widely utilized in material and life sciences. However, contrary to the rich chemistry of porphyrins and its related compounds, *i.e.* corroles and norcorroles, the structural diversity of phthalocyanine derivatives has been limited due to a scarcity of versatile synthetic methods, especially for modification of the *meso*-positions that are critical for their photophysical functionality.[1-2]

Herein we present a novel synthetic strategy and methodology for the *meso*-position editing of phthalocyanine derivatives through deprotonative macrocyclization of open-form acyclic phthalonitrile tetramer-metal complexes, which are obtained by thiolate-mediated reductive tetramerization of phthalonitrile and metalation.[3-4] To demonstrate the utility of this protocol, we synthesize several *meso*-*N*-edited phthalocyanine derivatives, including a 16π-electron antiaromatic nickel tetrabenzodiazanorcorrole, and 17π-electron paramagnetic tetrabenzotriazacorrole and tetrabenzodiazacorrole complexes. The unique electronic properties of these complexes, such as paratropicity and radical character, are characterized by both experimental and computational methods. The 16π-electron antiaromatic tetrabenzodiazanorcorrole undergoes skeletal transformations upon reactions with nucleophiles, resulting in the formation of nonaromatic and aromatic π-conjugates. Furthermore, the 17π-electron tetrabenzotriazacorroles and tetrabenzodiazacorroles display redox-induced aromaticity switching, highlighting the dynamic electronic nature of these macrocycles.

Phthalocyanine **meso-Edited Phthalocyanines**



Tetrabenzo diazanorcorrole | Tetrabenzo triazacorrole | Tetrabenzo diazacorrole

REFERENCES

1. J. Mack, N. Kobayashi, *Chem. Rev.* **2011**, *111*, 281.
2. M. O. Senge, N. N. Sergeeva, K. J. Hale, *Chem. Soc. Rev.* **2021**, *50*, 4730.
3. Y. Takiya, T. Saito, N. Toriumi, M. Uchiyama, *Nat. Commun.* **2025**, *16*, 3067.
4. T. Saito, Y. Takiya, N. Toriumi, M. Uchiyama, *submitted*.

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Subphthalocyanines: Nonplanar Aromatic Chiral Porphyrinoids

Tomas Torres[a,b,c], **Jorge Labella**[a], **Elisa López-Serrano**[a], **Marta Gómez-Gómez**[a], **Juan Laforga-Martín**[a], **Jorge Labrador-Santiago**[a,b], **Daniel Holgado**[a].

[a] *Departamento de Química Orgánica, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain.*
[b] *IMDEA-Nanociencia, c/Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain.*
[c] *Institute for Advanced Research in Chemical Sciences (IAdChem), 28049 Madrid, Spain.*

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Thanks to their outstanding structural and photophysical characteristics—including strong UV–vis and near-infrared (NIR) absorption and/or emission, excellent charge-transport behavior, and broad chemical tunability—subphthalocyanines (SubPcs) have emerged as one of the most thoroughly investigated and adaptable porphyrinoid families [1]. Their distinctive bowl-shaped, non-planar architecture endows them with exceptional versatility, enabling a variety of advanced applications. Among these are the generation of polar supramolecular assemblies, the development of thermotropic and lyotropic liquid-crystalline materials, and their implementation as non-fullerene acceptors. In this section, we explore the use of SubPcs in molecular photovoltaics [2], with particular attention to their role as singlet-fission materials [3], and consider the potential of enantiopure derivatives [4] for chiral technologies [5]. Additionally, we highlight recent progress in the synthesis and characterization of SubPc-based columnar materials [2] and discuss on-surface synthetic methodologies toward two-dimensional chiral polymers [4a].

[1] a) Lavarda, G.; Labella, J.; Martinez-Diaz, M. V.; Rodriguez Morgade, M. S.; Osuka, A.; Torres, T. Chem.Soc. Rev. 2022, 51, 9482. b) Labella, J.; Torres, T. Trends Chem. 2023, 5, 353.
[2] Labella, J.; Shoyama, K.; Guzmán, D.; Stolte, M.; Torres, T.; Würthner, F. ACS Mater. Lett. 2023, 5, 543.
[3] Gotfredsen, H.; Tykwinski, R.; Torres, T.; Clark, T.; Guldi, D. M. et al. J. Am. Chem. Soc. 2023, 145, 9548.
[4] a) Labella, J.; Lavarda, G.; Hernández, L.; Aguilar, F.; Díaz-Tendero, S.; Lobo-Checa, J.; Torres, T. J. Am. Chem. Soc. 2022, 144, 16579. b) Lavarda, G.; Tejerina, L.; Torres, T.; Martínez, M. V. Chem. Sci. 2024, 15, 19369.
[5] Labella, J.; Kumar Bhowmick, D.; Gupta, A.; Kumar, A.; Lopez, E.; Naaman, R.; Torres, T. Chem. Sci., 2025,16, 8783

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Effects of Dimerization on the Structure and Function of Membrane-bound Nitric Oxide Reductases

Takehiko Tosha[a]

[a]*Graduate School of Science, University of Hyogo, Japan*

ORALS

Regulation of the function of membrane-bound enzymes via oligomerization is one of the central topics in cell physiology. For example, the effects of the oligomerization the function of an aerobic respiration enzyme, cytochrome *c* oxidase (CcO), have been extensively studied. In contrast, little is known about how the oligomerization state affects the structure and function of anaerobic respiration enzymes, such as nitric oxide reductase (NOR), which catalyzes the reduction of NO to N_2O ($2NO + 2H^+ + 2e^- \Rightarrow N_2O + H_2O$) at a heme/non-heme iron active center. There are two types of NORs: quinol-dependent NOR (qNOR), which receives electrons from quinol for NO reduction, and cytochrome *c*-dependent NOR (cNOR), which uses cytochrome *c* as an electron donor. We previously found that qNOR from the pathogenic bacterium *Neisseria meningitidis* forms a dimer and exhibits higher NO reduction activity in the dimeric form than the monomeric form [1]. Here, to elucidate the origin of the higher enzymatic activity of dimeric qNOR and to understand the relationship between oligomerization state and enzymatic function in NORs, we determined the structures of the monomeric and dimeric NORs by single-particle cryo-electron microscopy (cryo-EM).

High-resolution structures of the highly active dimeric and less active monomeric forms of qNOR from *N. meningitidis* determined at a resolution of 1.89 and 2.25 Å, respectively, revealed the structural basis for the regulation mechanism of the enzymatic activity via oligomerization [2]. In the monomeric form, increased flexibility of helices near the dimer interface induced a conformational change in the essential residue Glu563 near the active site, although it is located apart from the dimer interface. Furthermore, the mutation of Glu563 to Ala disrupted its interactions with surrounding residues and increased the population of the monomeric form. These structural findings indicate that the active site and the dimer interface are connected through a network of interactions, providing insights into the regulation mechanism of the enzymatic function by the oligomerization. We also determined the structures of cNOR from *Pseudomonas aeruginosa* in both dimeric and monomeric states at resolutions of 2.1 and 2.5 Å, respectively, by cryo-EM. These structures revealed that the mode of dimerization in cNOR is completely different from that in qNOR, and that dimerization affects the coordination structure of heme in the active site of cNOR. To elucidate the impact of dimerization on the enzymatic function of cNOR, the functional studies on the dimeric cNOR are currently underway. In the presentation, the role of oligomerization state of NORs in the enzymatic function will be discussed.

REFERENCES

1. Jamali *et al. IUCrJ* (2020) 7, 404-415
2. Gopalasingam *et al. In revision*.

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Exploiting chromophores and inorganic nanomaterials in functional nanohybrids

Mariachiara Trapani[a], Maria Angela Castriciano[b], Massimiliano Cordaro[b], Antonino Mazzaglia[a], Andrea Romeo[b], Roberto Zagami[b], Luigi Monsù Scolaro[b]

[a]*CNR- ISMN (Istituto per lo Studio dei Materiali Nanostrutturati), URT Messina c/o Dip. CHIBIOFARAM, Università degli Studi di Messina, V. le Stagno d'Alcontres 31, 98166, Messina, Italy.* [b] *Dip. CHIBIOFARAM, Università degli Studi di Messina, V. le Stagno d'Alcontres 31, 98166, Messina, Italy.*

Nanostructured materials based on organic chromophores are widely investigated for sustainable technologies, including energy conversion, environmental applications, and (bio)sensing [1].
In this framework, considerable efforts from the scientific community have been devoted to developing functional hybrid nanoassemblies by integrating inorganic nanomaterials with organic dyes, a promising strategy for achieving enhanced properties and multifunctionality [2].
Here, hybrid supramolecular nanoarchitectures combining organic dyes, such as BODIPY or porphyrin derivatives, with inorganic nanostructures (i.e., semiconductor quantum dots, gold nanoparticles or clusters, and carbon nanotubes) are presented and investigated using spectroscopic techniques.
Synthetic routes based on supramolecular interactions between organic dyes, as monomers or aggregates, and inorganic components have been exploited.
BODIPY- functionalized CdSe quantum dots enable highly efficient Förster resonance energy transfer, which is crucial for light-harvesting and optoelectronic devices aimed at reducing energy losses [3].
Moreover, inorganic nanomaterials, such as metallic nanostructures or carbon nanotubes functionalized with porphyrins, exhibit optical absorption in the visible and near-infrared regions and remarkable photostability [4-5].
Through nanoscale molecular design and supramolecular engineering, guided by the arrangement and mutual orientations of the components, the nanohybrids could offer eco-friendly solutions, as they do not require highly demanding experimental procedures. Furthermore, tailored functionalities and optimized performance could be achieved through fine-tuning of nanomaterial properties and synergistic functional effects.
The approach highlights the high versatility of the nanoassemblies for multifunctional applications, including solar energy harvesting, photocatalysis, and the development of sensing platforms for environmental and health.

REFERENCES

1. A. S. Klymchenko, D. S. Biswas, P. Didier, Adv. Mater. 2025, 37, e01237
2. C. Sanchez, B. Julian, P. Belleville, M. Popall, J. Mater. Chem., 2005, 15, 3559–3592.
3. A. Panniello, M. Trapani, M. Cordaro, C. N. Dibenedetto, R. Tommasi, C. Ingrosso, E. Fanizza, R. Grisorio, E. Collini, A. Agostiano, M. L. Curri, M. Castriciano, M. Striccoli, Chem. Eur. J. 2021, 27(7), 2371-2380.
4. M.Trapani, M. Castriciano, A. Romeo, G. De Luca, N. Machado, B. D. Howes, G. Smulevich, L. Monsù Scolaro, Nanomaterials, 2019, 9, 1026.
5. M. Trapani, A. Mazzaglia, A. Piperno, A. Cordaro, R. Zagami, M. Castriciano, A. Romeo, L. Monsù Scolaro, Nanomaterials, 2020, 10, 669.

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The function and evolutionary diversity of chlorophyll biosynthetic enzymes that determine pigment specificity

Yusuke Tsukatani

Biogeochemistry Research Center, Japan Agency for Marine-Earth Science and Technology (JAMSTEC)

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Chlorophylls and bacteriochlorophylls are essential for harvesting light energy and driving photosystems. Phototrophic proteobacteria possess either bacteriochlorophyll (BChl) *a* or BChl *b* as their main pigment, depending on the species. Among naturally occurring pigments, BChl *b* is the sole pigment showing an absorption maximum in the near-infrared region. We have shown that chlorophyllide oxidoreductase (COR), a nitrogenase-like enzyme, possesses distinct substrate-recognition and catalytic mechanisms that determine whether the host species produces BChl *a* or *b*. We also unveiled a previously uncharacterized catalytic activity of BChl *a*-type COR—8-vinyl reduction, which is functionally replaced by BciA in some species. BchJ, the remaining Bch protein of unknown function, was found to enhance the catalytic activity of COR and is proposed to facilitate substrate channeling between pigment biosynthesis enzymes.

Geranylgeranyl reductase (GGR) catalyzes the hydrogenation of unsaturated hydrocarbons in isoprenoid compounds. GGRs in photosynthetic organisms typically perform successive triple hydrogenation to produce (B)Chl with a phytyl chain. We found that the γ-proteobacterium *Halorhodospira halochloris* possesses a unique GGR that catalyzes only double hydrogenation, producing BChls with a tetrahydrogeranylgeranyl tail. We also constructed a variant enzyme derived from *H. halochloris* GGR that performs only single hydrogenation. The results of this study provide new insights into the catalytic mechanisms of multi-position reductions by a single enzyme.
Together, these findings elucidate the functional roles of BchJ and COR in pigment specificity and reveal the catalytic plasticity of GGR. This work provides fundamental insights into the enzymatic mechanisms and evolutionary diversity of (bacterio)chlorophyll biosynthesis.

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Enzyme-responsive materials for photodynamic therapy

Sinem Tuncel Kostakoglu

Acibadem Mehmet Ali Aydinlar University, Faculty of Engineering and Natural Sciences, Department of Basic Sciences, Ataşehir, 34752 Istanbul, Türkiye

Photodynamic therapy (PDT) is a noninvasive cancer treatment that has gained attraction in recent years. However, its clinical use is limited by several issues, including hydrophobicity, poor targeting of photosensitizers (PSs), and hypoxia of the tumor microenvironment. Combining enzyme-responsive agents with PDT offers new aspects to overcome these challenges. Tumor tissues have a distinct enzymatic system compared to normal tissues, and abnormally expressed enzymes are potential targets for cancer therapy. PDT utilizes the properties of enzyme-responsive agents to deliver PSs to the target site and selectively release them, improving therapeutic outcomes [1]. Studies have shown that numerous enzymes are overexpressed in tumor tissues, exhibit excellent specificity and selectivity in binding and cleaving substrates, and exhibit rapid and efficient reactions. This offers new strategies for controlled and targeted drug delivery, enabling the selective delivery of PSs to tumor cells and tissues. The combination of PDT and enzyme-responsive materials can enhance the ability of PSs to actively target tumors, control PS release, increase drug accumulation in tumors, alleviate tumor hypoxia, and reduce systemic phototoxicity, thus significantly improving the therapeutic efficacy of PDT [2].

The presence of functional amine and carbonyl groups in the structure of barbituric acid allows the investigation of a wide variety of substituents to analyze the chemical structure-biological activity relationship [3]. It has the ability to form hydrogen bonds [4] with the active site of targeted enzymes, thus enabling various interactions with target biomacromolecules, including critical enzymes. In this work, it is aimed to prepare potential enzyme-responsive third-generation photosensitizers by combining the PS with a barbituric acid group. The molecular design is composed of the barbituric acid, which exhibits both fluorescence-quenching properties and can interact with enzymes or biomolecules through hydrogen bonds, are linked to the PS via ester or ether groups. The photophysical properties, self-assembly behavior and hydrolysis in the presence of esterase enzymes are investigated using spectroscopic methods.

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REFERENCES

1. Zhang H, Lin H, Su D, Yang D and Liu J. *Mol. Pharm.* 2022; **19**: 630-641.
2. Zhi S, Huang M and Cheng K. *Drug Discov. Today* 2024; **29**: 103965.
3. Ernst BJ, Clark GF and Grundmann O. *Current Pharm. Des.* 2015; **21**: 3681-3691.
4. Akyol B, Çokluk EM, Ayhan MM, Tuncel Kostakoğlu S and Gürek AG. *ACS Omega* 2025; **10**: 1716-1726.

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Dye-Degradation Reaction by Cytochrome P460 from *Nitrosomonas europaea*

Takeshi Uchida[a], Marika Yamaguchi[b], and Koichiro Ishimori[a]

[a]*Department of Chemistry, Faculty of Science, Hokkaido University*
[b]*Department of Chemistry, School of Science, Hokkaido University*

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Dye-decolorizing peroxidases (DyPs) are members of the heme-containing peroxidase superfamily. They catalyze the degradation of a variety of synthetic dyes such as anthraquinone and azo dyes through reactions with hydrogen peroxide (H_2O_2). Although these enzymes are considered promising for the bioremediation of diverse synthetic dyes commonly found in wastewater, their low-pH optimum for dye-decolorizing activity limits their practical use. The reaction is strongly pH dependent, with maximal activity observed around pH 4 [1]. In addition, functional expression in *Escherichia coli* is often inefficient, frequently resulting in inactive, heme-free forms. To circumvent these limitations, we focused on P460 from *Nitrosomonas europaea*, a *c*-type heme protein containing a covalently attached heme that exhibits guaiacol peroxidase activity under near-neutral conditions [2].

Recombinant P460 was expressed in *E. coli* with coexpression of pEC86, a protein system necessary for cytochrome *c* maturation. Its dye-decolorizing activity was evaluated by monitoring the degradation of Reactive Blue 19 (RB19) using absoprtion spectroscopy. P460 efficiently degraded RB19 at pH 8.0, retaining high activity under conditions where DyPs are inactive. P460 has one solvent-exposed tryptophan residue (Trp117), but it does not function well as a reaction center. Therefore, to degrade RB19 more efficiently, we engineered a surface radical site by substituting Ala47 (Fig. 1), a solvent-exposed residue proximal to the heme, with tryptophan (A47W), based on the long-range electron-transfer mechanism observed in DyPs [2]. The resulting A47W mutant exhibited a markedly enhanced initial degradation rate of 4.6 s^{-1} at 5 μM RB19, approximately 40-fold higher than that of the wild-type (WT, 0.12 s^{-1}). Kinetic analyses of the reaction with H_2O_2 revealed that, unlike WT P460, the A47W mutant did not form the high-valent two-electron oxidized species (Compound I); instead, only a one-electron oxidized species was detected (Fig. 2). These results indicate that electron transfer from the introduced tryptophan forms a tryptophan radical–a Compound ES-like intermediate observed in cytochrome *c* peroxidase–leading to the improvement in dye-decolorizing activity. Our findings demonstrate that P460 overcomes the pH limitations of DyPs, while rational engineering successfully imparts potent activity toward bulky dyes. This suggests that the P460 platform could lead to the realization of an effective *E. coli*-based dye-decolorizing system.

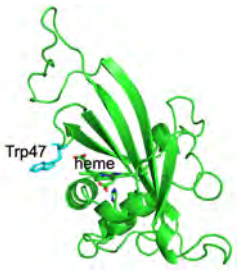


Fig. 1 AlphaFold3-predicted model structure of P460

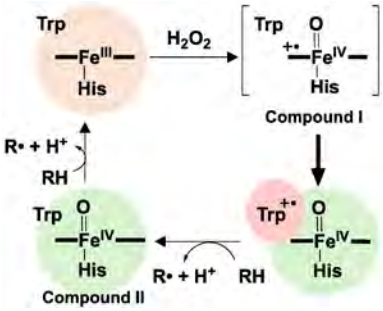


Fig. 2 Proposed reaction mechanism of the A47W mutant upon reaction with H_2O_2.

REFERENCES

1. Uchida et al., (2015) *Biochemistry*, **54**, 6610–6621.
2. Liew et al., (2020) *Biochemistry*, **59**, 704–716.
3. Uchida et al., (2021) *J. Inorg. Biochem.*, **219**, 111422.

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Development of $FePc(CO_2H)_8$-Catalyzed Oxidative Chemical Modification of Glycine Derivatives

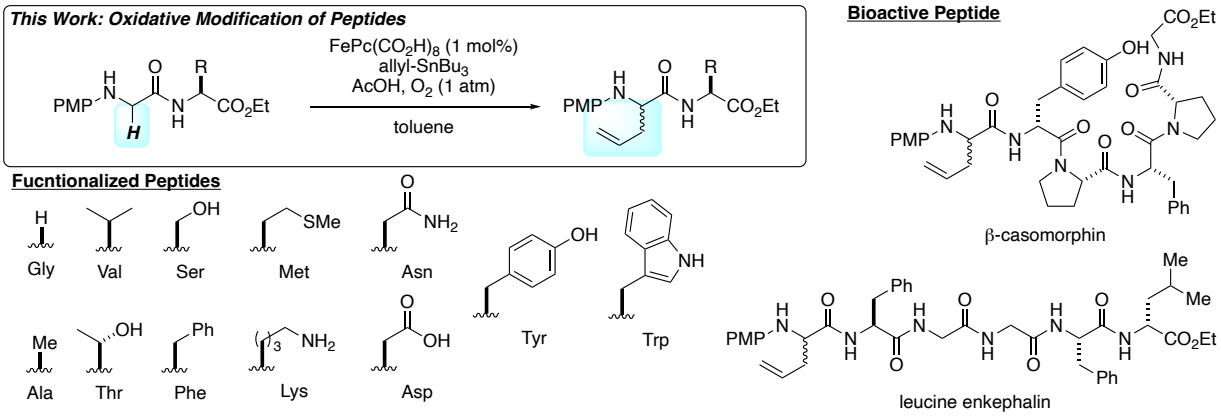
Hirofumi Ueda[a], Kei Yoshida[a], Mirai Hayashi[a], Nagao Kobayashi[b], Hidetoshi Tokuyama[a]

[a] *Graduate School of Pharmaceutical Sciences, Tohoku University*
[b] *Graduate School of Sciences, Tohoku University*

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Since peptides are biomolecules involved in various biological processes, considerable efforts have been devoted in recent years to developing chemical modification methods of amino acids and peptides for the elucidation of their functions and the creation of peptide-based therapeutics.[1-2] However, challenges in chemoselectivity and regioselectivity often arise because the peptidess possess acidic protons and various functional groups derived from amino acids. As a result, many current methods are limited to simple amino acid derivatives, peptides with aliphatic side chains, or peptides with protected functional groups.

Recently, our group developed an oxidative dimerization reaction targeting tryptophan derivatives by employing an octacarboxy iron phthalocyanine ($FePc(CO_2H)_8$) complex[3] that mimics the function of the enzyme P450.[4] By combining catalytic amounts of $FePc(CO_2H)_8$ with molecular oxygen, the oxidative reaction proceeds with high chemoselectivity without the need to protect amino acid–derived functional groups. Inspired by the high chemoselectivity and oxidative capability of this catalytic system, we developed an oxidative modification of peptides targeting glycine residues. Through extensive investigations, we found that various glycine derivatives, including unprotected dipeptides and unbioactive oligo-peptides, undergo oxidative transformation under an oxygen atmosphere with catalytic amounts of $FePc(CO_2H)_8$ in the presence of nucleophiles to afford the corresponding adducts in the good yields. In this presentation, we will report the optimization of reaction conditions and the substrate scope of this oxidative modification method.



REFERENCES

1. Peng, K.; Dong, Z.-B. *Adv. Synth. Catal.* **2021**, *363*, 1185.
2. Brimble, M. A.; Noisier, A. F. M. *Chem. Rev.* **2014**, *114*, 8775.
3. Okada, Y.; Kobayashi N. *J. Inorg. Biochem.* **2025**, *262*, 112737.
4. Ueda, H.; Sato, S.; Noda, K.; Hakamata, H.; Kwon, E.; Kobayashi, N.; Tokuyama, H. *Angew. Chem. Int. Ed.* **2023**, *62*, e20230240.

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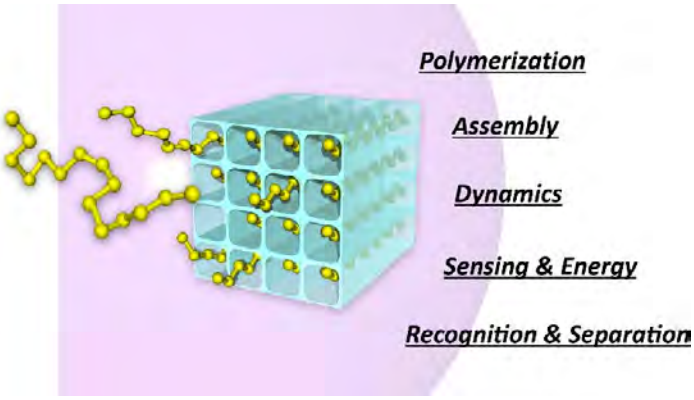


Reticular Frameworks for Macromolecular Science and Technology

Takashi Uemura[a]

[a]Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

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Reticular frameworks (RFs) have been successfully applied in numerous domains, including storage and separation, catalysis, energy, and sensing. However, the majority of RF studies focused on gas and solvent molecules as guests, despite the potential of infinite nanochannel structures for the encapsulation of macromolecules. RFs, characterized by their crystalline porous structures and tunable properties, have significant advantages in polymer production and functionalization, improving their synthetic efficiency, structural regularity, stability, conductivity, mechanical properties, and overall performance through a combination of structural characteristics[1].

Ordered nanopores in RFs act as structural scaffolds, guiding polymerization and depolymerization with spatial precision and enabling control over macromolecular structures and arrangement[2]. RFs exhibit exceptional potential for macromolecular recognition and separation, affording scalable platforms for highly selective processing, purification, and recycling[3]. Synergistic coupling of reticular chemistry with polymer engineering opens new avenues for the design of next-generation functional materials[4]. The rapid progress in this field has led to breakthroughs in both fundamental science and materials applications, promoting investigations to expand their potential in creating advanced materials and realizing chemical circulation systems.

REFERENCES

1. (a) *Adv. Mater.* **2025**, e14489. (b) *Coord. Chem. Rev*. **2022**, *466*, 214601. *Acc. Chem. Res.* **2021***, 54,* 3593. (c) *Matter* **2020***, 3*, 652.
2. (a) *Nat. Commun.* **2018**, *9*, 329. (b) *J. Am. Chem. Soc.* **2019**, *141*, 19565. (c) *Nat. Commun.* **2020**, *11*, 3573. (d) *J. Am. Chem. Soc*. **2020**, *142*, 5509. (e) *J. Am. Chem. Soc.* **2023**, *145*, 2448. (f) *Nat. Synth.* **2023**, *2,* 848. (g) *Nat. Commun.* **2025**, *16*, 6948.
3. (a) *Nat. Commun.* **2018**, *9*, 3635. (b) *J. Am. Chem. Soc.* **2020**, *142*, 3701. (c) *Angew. Chem. Int. Ed.* **2021**, *60*, 11830. (d) *Chem* **2023**, 9, 2817. (e) *J. Am. Chem. Soc.* **2024**, *146*, 16369. (f) *J. Am. Chem. Soc.* **2025**, *147*, 17228. (g) *Angew. Chem. Int. Ed.* **2025**, e202513518. (h) *J. Am. Chem. Soc.* **2026**, *148*, *in press.*
4. (a) *J. Am. Chem. Soc.* **2017**, *139*, 7886. (b) *Nat. Commun.* **2018**, *9,* 1660. (c) *J. Am. Chem. Soc.* **2019**, *141,* 14549. (d) *Angew. Chem. Int Ed.* **2021**, *60*, 17947. (e) *Nat. Commun.* **2023**, *14,* 3241.

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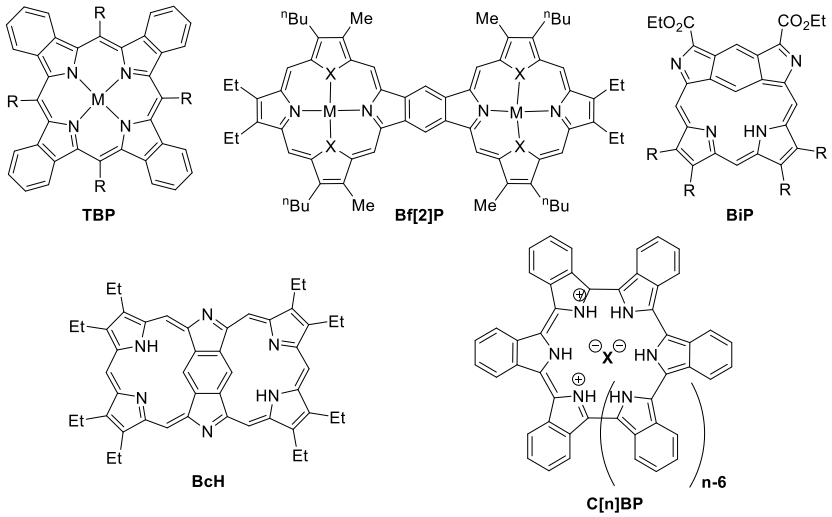
Benzene-Fusion of Porphyrinoids. Synthesis and Effects on Their Optical Properties

Hidemitsu Uno

School of Science and Engineering, Ehime University, 3-5 Bunkyo-cho, Matsuyama 790-8577, Japan

ORALS

We have been engaged in projects concerned with synthesis of π-expanded porphyrinoids and elucidation of their properties, since we reported the synthesis of tetrabenzoporphyrins (**TBP**s) based on the *retro*-Diels-Alder reaction of bicyclo[2.2.2]octadiene (BCOD) moieties.[1] During the projects, we have developed the efficient pericyclic cycloreversion reactions of dihydroxyBCOD, dioxoBCOD, and oxobicyclo[2.2.1]heptadiene. Utilization of these reactions to precursors in the final stage of synthesis enabled us to prepare a variety of π-conjugated compounds so far difficult to prepare in pure forms. The precursor molecules were easily purified by usual methods such as column chromatography and/or recrystallization, although rather tedious preparation schemes were required. As we had the method to introduce benzene rings into porphyrinoid molecules, we succeeded in the preparation of benzene-fused cyclo[n]pyrroles (**C[n]BP**),[2] oligoporphyrins (**Bf[n]P**),[3] benzene-inserted porphyrinoid (**BiP**),[4] and benzene-crosslinked hexaphyrin (**BcH**)[5] and elucidation of their spectroscopic properties. In my talk, preparation and optical properties of these compounds will be discussed as well as aromaticity and antiaromaticity enhanced by fusion of benzene rings at β-positions of porphyrinoids.



1. Okujima T.; Ando C.; Agrawal S.; Matsumoto H.; Mori S.; Ohara K.; Hisaki I.; Nakae T.; Takase M.; Uno H.; Kobayashi N. *J. Am. Chem. Soc.* **2016**, *138*, 7540; Okujima T.; Jin G.; Matsumoto N.; Mack J.; Mori S.; Ohara K.; Kuzuhara D.; Ando C.; Ono N.; Yamada H.; Uno H.; Kobayashi N.; *Angew. Chem. Int. Ed.* **2011**, 50, 5699.
2. Ito S.; Murashima T.; Uno H.; Ono N.; *J. Chem. Soc., Chem. Commun.*, **1998**, 1661.
3. Uno H.; Tagawa K.; Mori S.; Okujima T.; Takase M.; Nakae T. *Bull. Chem. Soc. Jpn.*, **2017**, *90*, 1375; Kim P., Ham S.; Oh J.; Uoyama H.; Watanabe H.; Tagawa, K; Uno H; Kim D.; *Phys. Chem. Chem. Phys.*, **2013**, *15*, 10612; Uoyama, H.; Kim K. S.; Kuroki K.; Shin J.-Y.; Nagata, T.; Okujima T.; Yamada H.; Ono N.; Kim D.; Uno H. *Chem. Eur. J.* **2010**, *16*, 4063.
4. Uno H.;Muramatsu K.; Hiraoka S.; Tahara H.; Hirose M.; Tamura E.; Shiraishi T.; Mack J.; Kobayashi N.; Mori S.; Okujima T.; Takase M. *Chem. Eur. J.* **2020**, *26*(25), 5701.
5. Uno, H.; Hata, S.; Hashimoto, K.; Muramatsu, K; Nakano, H.; Takiue, T.; Uoyama, H; Mori, S.; Okujima, T.; Takase, M. *J. Porphyrins Phthalocyanines*, **2023**, *27*, 1382.

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Development of Novel Small Molecule-based Theranostics Technologies for Cancer

Yasuteru Urano[a,b]

[a]*Graduaste School of Pharmaceutical Sciences, The University of Tokyo*
[b]*Graduaste School of Medicine, The University of Tokyo*

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Our research group has been working for more than 20 years on the logical design and development of small molecule-based photo-functional probes that function under visible light without causing damage to cells and animals. We have established some new principles for controlling fluorescence, such as photoinduced electron transfer and intramolecular spirocyclization, and based on these strategies, novel highly functional probes, such as self-blinking fluorescent probes for live super-resolution imaging and fluorescent probes for real-time quantification of glutathione concentration in living cells, as well as caged compounds that functions by the yellow light illumination to control C. elegans behavior were successfully developed.
Many probes including those for super-resolution imaging in living cells, for quantification of intracellular concentration of biological thiols such as gluhatione, and for rapid cancer imaging during operation have been successfully developed. They were achieved for the first time by chemically precise design of probes, which have an extremely large contribution for the future biology and medicine.
In my talk, our recent progress in chemistry-based medical technology for intraoperative cancer detection will be showcased. First, we succeeded in preparing a library of fluorogenic probes composed of more than 400 probes for various amino- and dipeptidylpeptidases. By applying them to the cancerous and normal regions of freshly resected human cancer samples, novel specific biomarker enzymatic activities for several tumors were successfully found out and identified. For example, by this approach, dipeptidyl peptidase-4 (DPP-4) activity was found to be selectively upregulated in esophageal cancer compared to surrounding normal sites, and the tumor region in the resected human fresh specimens was clearly visualized by topically spraying DPP-4-activatable fluorescence probes within a few minutes. To date, a first-in-human study recruiting six patients has been completed, and a human phase II clinical trial is currently underway in Japan.
Furthermore, we recently started to expand imaging modality to radionuclide imaging such as SPECT and PET for deeply-located tumors, and also to establish novel cancer theranostics technologies by developing prodrug-type and radiotherapeutic anticancer drugs which will realize personalized and precision medicine based on the biomarker enzymatic activity of each patient. In my talk, the latest results of the development of various small molecule-based imaging probes and therapeutic drugs based on the latest chemistry and its medical applications to realize new theranostics for various types of cancers will be also showcased.

REFERENCES

1. Nakadate M, et al., ***J. Am. Chem. Soc.***, 147: 30684-30693, 2025.
2. Kuriki Y, et al., ***J. Am. Chem. Soc.***, 146: 521-531, 2024.
3. Kuriki Y, et al., ***Chem. Sci.***, 13: 4474-4481, 2022.
4. Tachibana R, et al., ***Commun. Chem.***, 3: 82, 2020.
5. Fujita K, et al., ***ACS Cent. Sci.***, 6: 2217–2227, 2020.
6. Umezawa K, et al., ***Nat. Chem.***, 9: 279-286, 2017.
7. Uno SN, et al., ***Nat. Chem.***, 6: 681-689, 2014.
8. Urano Y, et al., ***Sci. Transl. Med.***, 3:110ra119, 2011.
9. Urano Y, et al., ***Nat. Med.***, 15: 104-109, 2009.

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On-Surface Synthesis of Carbahemiporphyrazine-Based Polymers

José Ignacio Urgel[a]

[a]*IMDEA Nanociencia, C/ Faraday 9, Campus de Cantoblanco, Madrid, 28049*

Porphyrinoid chemistry has long provided a versatile platform for designing functional molecular nanostructures, attracting sustained interest in surface science due to the tunable electronic, optical, and catalytic properties of these macrocycles. Within this broad family, hemiporphyrazines, porphyrinoids composed of mixed pyrrolic and benzenoid (or pyridinic) units, are underexplored systems. Their reduced symmetry, atypical nitrogen content, and inherent conformational flexibility give rise to unusual frontier-orbital distributions and coordination motifs that deviate from those of classical tetrapyrrolic macrocycles. These features make hemiporphyrazines compelling candidates for surface-assisted synthesis, metalation, and integration into low-dimensional architectures, where their distinct reactivity and coordination behavior can be harnessed.

In this context, I report the on-surface fabrication and atomically resolved characterization of a series of exotic carbahemiporphyrazine derivatives containing six- and seven-nitrogen macrocycles, designed with isopropyl substituents to promote controlled covalent coupling [1]. Three precursors (P1, P2, and P3) were deposited on Au(111) and investigated under ultrahigh-vacuum conditions using scanning tunneling microscopy (STM), non-contact atomic force microscopy (nc-AFM), and ab initio modeling. P1 and P2 feature macrocycles comprising two pyrroles and two benzene units, while P3 incorporates a pyridine ring in place of one benzene, increasing the nitrogen content. Thermal activation triggered a surface-assisted [3+3] cycloaromatization of the isopropyl groups, yielding atomically precise covalently linked architectures, including dimers (0D), as well as extended 1D and 2D polymeric networks. Subsequent exposure of these free-base macromolecules to a flux of Co atoms enabled the formation of cobalt-metalated species. Remarkably, the dicarbahemiporphyrazines 1 and 2 exhibit metal coordination exclusively to the two pyrrolic nitrogens, distinct from the canonical fourfold coordination in porphyrins, whereas monocarbahemiporphyrazine 3 shows a threefold coordination environment.

This examples reveal how macrocycle composition and dimensionality govern metal-binding motifs and electronic properties. Overall, this on-surface synthetic strategy provides a robust route to tailor-made carbahemiporphyrazine architectures and opens pathways for exploring metalated low-coordinated porphyrinoid systems with potential applications in molecular electronics and catalytic model studies.

REFERENCES

1. On-Surface Synthesis of Covalently-Linked Carbaporphyrinoid-Based Low-Dimensional Polymers. A. Barragán, M. Urbani, A. Gallardo, E. Pérez-Elvira, Ó. Jover, K. Lauwaet, J. M Gallego, R. Miranda, M. Di Giovannantonio, D. Écija, T. Torres, J. I Urgel. Small 21 (2) 2408085 (2025).

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Topological control in polymersome-based nanomedicine

Jan C.M. van Hest[a], Shukun Li, Jingxin Shao, Yingtong Luo, Yudong Li, Hanglong Wu, Shoupeng Cao

[a]*Eindhoven University of Technology, Department of Biomedical Engineering, Institute for Complex Molecular Systems, PO Box 51,3 5600 MB Eindhoven, The Netherlands; email j.c.m.v.hest@tue.nl*

The efficacy of nanoparticles employed in drug delivery is affected by a range of features such as their size, surface properties and shape. Over the past years we have developed methods to construct polymer vesicles, or polymersomes, with a range of different topologies. In this lecture topologically controlled nanoparticles will be discussed with photodynamic and photothermal (PDT/PTT) features, which are used in cancer treatment. In a first example poly(ethylene glycol)-poly(D,L-lactic acid) block copolymers are created, which are assembled in a range of topologies, from micellar worms to vesicles and bowl-shaped architectures known as stomatocytes. During the assembly process, phthalocyanine (Pc) is included as PDT active component. A detailed *in vitro* and *in vivo* study shows that the topology both affects Pc efficiency and in vivo biodistribution, showing that worms and stomatocytes are the most effective carrier systems for PDT in a tumor model [1]. In a second example, aggregation-induced emission (AIE) moieties based on tetraphenyl ethylene are included in the hydrophobic part of a diblock copolymer composed of poly(ethylene glycol)-poly(trimethylene carbonate). This allows us to create polymersomes with inherent fluorescence and PDT. By creating anisotropy in the polymersome structure, not only therapeutic efficacy is installed, but also the propensity of the particles to act as nanomotors. This leads to an improved activity and deeper tissue penetration [2]. To ensure that these particles display mainly photothermal features, we furthermore have included a photothermal agent (PTA), which shows structural similarity with the AIE components but is excited with NIR irradiation. It converts the excited state predominantly in heat. Remarkably, despite the structural similarity with the AIE moieties, phase separation of the PTA is observed, leading to polymer vesicles with a "snowman" type of morphology, which both show excellent photothermal features as well as motile behavior [3].

REFERENCES

1. Li, S.; Li, Y.; Shen, G.; Sun, J.; Abdelmohsen, L.; Yan, X.; van Hest, J.C.M. Flexible Morphological Regulation of Photothermal Nanodrugs: Understanding the Relationship between the Structure, Photothermal Effect, and Tumoral Biodistribution. *ACS Nano* **2025**, *19* (2), 2799-2808. DOI: 10.1021/acsnano.4c15587.
2. Cao, S.; Shao, J.; Wu, H.; Song, S.; De Martino, M. T.; Pijpers, I. A. B.; Friedrich, H.; Abdelmohsen, L. K. E. A.; Williams, D. S.; van Hest, J. C. M. Photoactivated nanomotors via aggregation induced emission for enhanced phototherapy. *Nature Communications* **2021**, *12* (1), Article. DOI: 10.1038/s41467-021-22279-w.
3. Shao, J.; Luo, Y.; Wu, H.; Wang, J.; Zhou, X.; Er, S.; Cao, S.; Sun, H.; Garza, H.; Zheng, H.; Abdelmohsen, L. K. E. A.; van Hest, J. C. M. Designing polymersomes with surface-integrated nanoparticles through hierarchical phase separation. *Nature Communications* **2025**, *16* (1). DOI: 10.1038/s41467-025-57711-y.

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Thermal Dissipation of Absorbed Light in a Photo-Induced Enzymatic Reaction in the Cells of *Phaeodactylum tricornutum* via a *trans-cis* Isomerization in the Xanthophyll Cycle

Constantinos Varotsis[a], Charalambos Tselios[a], Charalambos Andreou[a], Vasiliki Valianti[b], and Eftychia Pinakoulaki[b]

[a]*Department of Chemical Engineering, Cyprus University of Technology,* 3603 *Limassol, Cyprus*
[b]*Department of Chemistry, University of Cyprus, 2109 Aglantzia, Cyprus*

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Cis-trans isomerizationis a fundamental molecular process essential for photobiological function. The marine pennate diatom *Phaeodactylum tricornutum* experiences specific light environments that trigger a cascade of events involving the *Lhcx* proteins which are essential for the non-photochemical quenching of Chl *a* fluorescence (NPD) and the xanthophyll cycle where diadinoxanthin (Dd) is converted in a high intensity light photoenzymatic reaction to diatoxanthin (Dt). We have performed a series of time-depended resonance Raman measurements on cells of *Phaeodactylum tricornutum* under different light intensity conditions and record spectra during the all-*trans* Dd to Dt transition in which the diadinoxanthin de-epoxidase (DDE) removes an epoxy group from Dd, converting it to Dt, at ambient temperatures. The observed spectral fingerprints of Dt are accompanied by two C=C modes at 1550 and 1565 cm^{-1} which originate from two distinct *cis*-Dts conformations of different origin. The conformer with the ν(C=C) at 1565 cm^{-1} contributes to the transition from light harvesting all *trans*-Dd to photoprotection *cis*-Dt.

REFERENCES

1. C. Tselios, Varotsis, C. Evidence for a reversible light-dependent transition in the photosynthetic pigments of diatoms *RSC Adv.*, 23, (2022) 31555-31563.
2. C. Andreou, Tselios, C., A. Ioannou, A., Varotsis, C. Probing the Fucoxanthin-Chlorophyll a/c-Binding proteins (FCPs) of the Marine diatom *Fragilariopsis sp*. by Resonance Raman spectroscopy *J. Phys. Chem. B*, 127 (2023) 9014-9020.
3. C. Andreou, C. Varotsis. Light harvesting and photoprotective states in the marine diatom *Fragilariopsis* sp.: functional implications of chlorophylls c_1/c_2 in the fucoxanthin–chlorophyll *a*/*c*-binding proteins (FCPs) *RSC Adv.*, *15*, (2025) 4322.

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Fluorescent probes for translational bioimaging

Marc Vendrell

Centre for Inflammation Research and IRR Chemistry Hub, Institute for Regeneration and Repair (IRR), The University of Edinburgh, EH16 4UU, Edinburgh, UK. Email: marc.vendrell@ed.ac.uk

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Fluorescent, activatable probes are valuable tools for live-cell imaging due to their tunability and target specificity.[1] Over the last few years, our group has designed a collection of fluorogenic amino acids and peptides for high-resolution biological imaging and translational medicine. Our team has demonstrated that this approach can be used to generate probes to visualize infection and immune cells in human biosamples,[2] *in vivo*[3] and in *ex vivo* human biopsies.[4] We have designed fluorescent amino acids to: 1) be compatible with conventional solid-phase peptide synthesis, 2) maintain the biomolecular recognition features of the native peptides, and 3) emit fluorescence preferentially after target binding, improving signal-to-noise ratios for imaging. Recently, we have included the smallest turn-on fluorescent amino acids for peptide-PAINT imaging and super-resolution microscopy,[5] and fluorogenic tags for proteins associated with immune cell function like interleukins,[6] immunophilins and chemokines[7] as well as nanobodies and antibodies.[8] Finally, the talk will also briefly discuss our efforts to establish these fluorescent probes for clinical applications.

REFERENCES

1. Cheng, Z. et al. Nat. Rev. Chem. **2020**, 4, 275.
2. a) Mendive-Tapia, L. et. al. Nat. Commun. **2016**, 7, 10940; b) Mendive-Tapia, L. et. al. Nat. Protoc. **2017**, 12, 1588; c) Mendive-Tapia et al. Angew. Chem. Int. Ed. **2022**, 61, e202117218.
3. a) Barth N. et al. Nat. Commun. **2020**, 11, 4027; b) Kaplaneris, N. et al. Nat. Commun. **2021**, 12, 3389; c) Subiros-Funosas, R. et. al. Chem. Sci. **2020**, 11, 1368; d) Barth N. et al. Angew. Chem. Int. Ed. **2022**, 61, e20211302.
4. a) Scott, J. et al. Nat. Commun. **2022**, 13, 2366. b) Scott, J. et al. Nat. Biomed. Eng. **2025**, *accepted*.
5. De Moliner et al. Angew. Chem. Int. Ed. **2023**, 62, e202216231.
6. Reese et al. ACS Cent. Sci. **2024**, 10, 143.
7. a) Bertolini et al. ACS Cent. Sci. **2024**, 10, 969; b) Bertolini et al. JACS **2024**, 146, 30565.
8. a) Kuru et al. Nat. Commun. **2024**, 15, 7531; b) Nadal-Bufi et al. JACS **2025**, 147, 7578.

About the Speaker

Marc Vendrell is Professor of Translational Chemistry and Biomedical Imaging at the College of Medicine and Veterinary Medicine in Edinburgh. His team has pioneered the design of smart chemical fluorophores for high-resolution optical imaging (>150 papers) and built an ambitious research programme linking physical and biomedical sciences through competitive funding -over £10M as PI (>£40M as co-I), including prestigious European ERC Consolidator and EIC Transition grants. Vendrell is co-inventor of 12 patents, PI for 9 licensed technologies and collaborative projects with industry and Pharma, and he has contributed to founding two spin-out companies on therapeutics (InPepcide) and diagnostics (IDxSense). Vendrell has a strong record of mentoring and training the next generation of translational scientists, with several alumni holding independent positions in academia and industry. He has won some awards and distinctions, the latest being the Bader Prize for eminence in Organic Chemistry by The Royal Society of Chemistry in 2023, and was elected Fellow of the Royal Society of Edinburgh, the Scottish national academy, in 2024. Vendrell currently heads the IRR Chemistry Hub at the College of Medicine in Edinburgh as one of the first global hubs for collaborative non-siloed chemical research to catalyse innovation in biomedical sciences and accelerate translational outputs.

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Photophysical properties of porphyrin-based Type-I and Type-II photosensitizers

Barbara Ventura[a]

[a]*Istituto per la Sintesi Organica e la Fotoreattività (ISOF) – Consiglio Nazionale delle Ricerche (CNR) – Via P. Gobetti, 101 – 40129 Bologna – Italy. E-mail: barbara.ventura@cnr.it*

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Porphyrins are extensively studied photosensitizers for photodynamic therapy, thanks to their ability to absorb light in the red/near-infrared region and to efficiently generate singlet oxygen, *via* triplet energy transfer to molecular oxygen (Type-II mechanism). In photodynamic therapy (PDT), however, the search for Type-I photosensitizers, i.e. generating reactive oxygen species (ROS) through an electron transfer process, is on the rise, since their mechanism of action is less oxygen-dependent and they can be employed in hypoxic environments, such as those of solid tumors [1]. It is thus highly important to develop porphyrin-based photosensitizers that can afford both Type-I and Type-II mechanisms.

In collaboration with the group of Prof. V. Heitz (University of Strasbourg), we recently investigated guanidinium-porphyrin derivatives as Type-I photosensitizers and a bisacridinium-porphyrin conjugate (Figure 1) as a system able to generate both Type-I and Type-II ROS. The latter was shown to undergo, in organic media, an ultrafast electron transfer from the porphyrin to the acridinium unit [2], similarly to other acridinium-porphyrin conjugates investigated by our groups [3-5]. Interestingly, in aqueous media, the charge-recombination process slows-down, allowing for long lived radicals able to generate Type-I ROS.

The photophysical properties of all the investigated systems, characterized by means of steady-state and time-resolved techniques, will be presented, as well as their possible application in PDT scenarios.

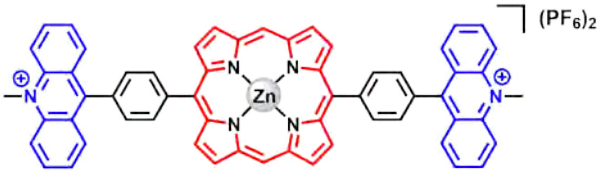


Figure 1. Chemical structure of the studied Zn(II)-porphyrin bis-acridinium conjugate.

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REFERENCES

1. M. Li, J. Xiong, Y. Zhang, L. Yu, L. Yue, C. Yoon, Y. Kim, Y. Zhou, X. Chen, Y. Xu, X. Peng, J. S. Kim, *Chem. Soc. Rev.*, **2025**, *54*, 7025.
2. A. Edo-Osagie, D. Sánchez-Resa, D. Serillon, E. Bandini, C. Gourlaouen, H.-P. Jacquot de Rouville, B. Ventura, V. Heitz, *C. R. Chim.* **2021**, *24*, 1.
3. F. Ruani, A. Edo-Osagie, H.-P. Jacquot de Rouville, V. Heitz, B. Ventura, N. Armaroli, *J. Porphyr. Phthalocyanines* **2023**, *27*, 569.
4. A. Edo-Osagie, D. Serillon, F. Ruani, X. Barril, C. Gourlaouen, N. Armaroli, B. Ventura, H.-P. Jacquot de Rouville, V. Heitz, *J. Am. Chem. Soc.* **2023**, *145*, 10691.
5. F. Ruani, D. Veclani, D. Sanchez-Resa, A. Edo-Osagie, G. Creste, A. Barbieri, V. Heitz, H.-P. Jacquot de Rouville, N. Armaroli, B. Ventura, *Chem. Eur. J.* **2025**, e02604, DOI: 10.1002/chem.202502604.

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Advances in the Development of Topical Phospholipid Carriers for Porphyrinic Photosensitizers

Martina Vermathen[a]

[a]*Department of Chemistry, Biochemistry, and Pharmaceutical Sciences, University of Bern, Bern, Switzerland*

ORALS

Topical Photodynamic Therapy (tPDT) using the porphyrin precursor 5-ALA is a widely used and well-accepted treatment modality of skin diseases. [1] To take advantage of newly developed porphyrinic photosensitizers (PSs) that can be tailored for specific targets [2], their direct application via the skin would be required for tPDT. However, this is still hampered by the lack of suitable, efficient topical carriers. [3]

Our research has focused on phospholipid bicelles [4] to examine their potential as novel carriers for tPDT. This contribution presents systematic studies in the development of bicelle-carriers with controllable size, morphology, internal structure, and stability. The capability to encapsulate porphyrinic PSs will be presented, as will their versatility, covering a broader range of PS structures. In this respect, our analytical approach, applying—among other methods—NMR spectroscopy, has proved a powerful tool for obtaining detailed information on PS encapsulation, localization at the carrier interface, and the dynamic properties of both the carrier and its payload. [5].

Skin penetration experiments were performed to assess the carrier's efficiency in delivering PSs into the outer skin layers. For this, various skin models, including 3D artificial human skin, were used for testing, thereby further complying with the 3R-principle. The use of excipients alongside the carrier and approaches to gain mechanistic insights into potential interactions with the skin lipid matrix will also be discussed.

REFERENCES

1. Morton C.A., Szeimies R.-M., Basset-Séguin N., Calzavara-Pinton P.G., Gilaberte Y., Hædersdal M., Hofbauer G.F.L., Hunger R.E., Karrer S., Piaserico S., Ulrich C., Wennberg A.-M., Braathen L.R. *J Eur Acad Dermatol Venereol*, 34 (2020), 17–29. DOI: 10.1111/jdv.16044
2. Akbar A., Khan S., Chatterjee T., Ghosh M. *J Photochem Photobiol, B: Biology* 248 (2023) 112796. doi.org/10.1016/j.jphotobiol.2023.112796
3. Lopez-Vidal L., Juskaite K., Ramöller I.K., Real D.A., McKenna P.E., Priotti J., Donnelly R.F., Paredes A.J. *Therapeutic Delivery*, 16, No. 3 (2025), 285–303. doi.org/10.1080/20415990.2024.2437978
4. Barbosa-Barros L., Rodríguez G., Barba C., Cócera M., Rubio L., Estelrich J., López-Iglesias C., de la Maza A., López O. *Small*, 8, No. 6 (2012), 807–818. doi: 10.1002/smll.201101545
5. Gjuroski I., Furrer J., Vermathen M. *Molecules* 26 (2021) 1942. doi.org/10.3390/molecules26071942

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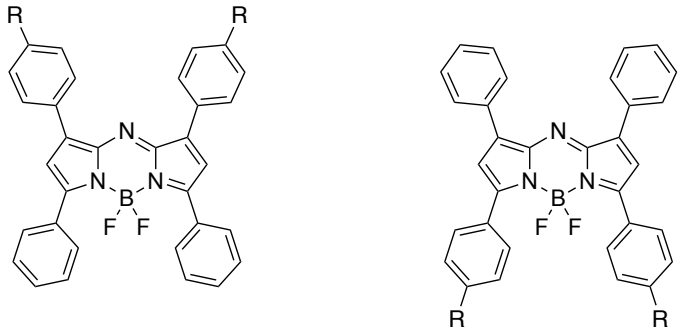
Synthesis and Properties of 1,3,5,7-Tetraphenyl-aza-BODIPYs Functionalized with Electron-withdrawing or Donating Groups

Maria da Graça H. Vicente[a], **Simran Dhingra**,[a] **Mistura O Olajuwon**,[a] **Petia Bobadova**,[b] **Frank Fronczek**[a] **and Kevin M. Smith**[a]

[a]*Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803*
[b]*Department of Chemistry and Fermentation Sciences, Appalachian State University, Boone, NC 28608*

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The 1,3,5,7-tetraphenyl-aza-BODIPY scaffold provides an ideal platform for developing near-infrared (NIR) fluorophores with emissions in both the NIR-I (700-950) and the NIR-II (>1000 nm) regions.[1] A simple strategy to red-shift the absorption and emission wavelengths of these aza-BODIPYs is the introduction of electron-withdrawing and/or electron-donating groups at specific positions. I will present recent work from our laboratory on the synthesis and investigation of two series of aza-BODIPYs, bearing electron-donating ($-NH_2$) or electron-withdrawing (NO_2, $-NH_3^+$, -N=C=S) groups at the *para*-positions of the phenyl groups,[2] and on the conjugation of the bisNCS derivatives with peptides.



R = NO_2, NH_2, NH_3^+, NCS

REFERENCES

1. Tajani, W.; Verrieux, L.; Sickinger, A.; Godard, A.; Rouillon, J.; Goze, C.; Dalonneau, F.; Rousselin, Y.; Maury, O.; Sancey, L.; Andraud, C.; Le Guennic, B.; Fihey, A.; Bodio, E. Available at SSRN: https://ssrn.com/abstract=5113194 or http://dx.doi.org/10.2139/ssrn.5113194.
2. S. Dhingra, M. O. Olajuwon, M. Al Horani, S. Al Horani, P. Bobadova-Parvanova, D. J. LaMaster, F. R. Fronczek and M. G. H. Vicente. *Dyes & Pigments* **2025**, 244, 113144.

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Active-Site Identity and Mechanistic Pathways in Porphyrin-Based Electrocatalysts for Water Splitting

Dino Villagrán[a], Nedy Ocuane, Alexandria Castillo, Rebeca Favela, Nasim Jafari

[a]*Department of Chemistry and Biochemistry, The University of Texas at El Paso*

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Macrocyclic porphyrins and phthalocyanines provide a versatile platform for probing structure–activity relationships in electrocatalytic water splitting, spanning homogeneous, heterogeneous, and polymeric architectures. This talk will examine how electronic structure, metalation, and extended frameworks govern hydrogen and oxygen evolution reactivity in porphyrin- and phthalocyanine-based systems. Metal-free and metallated macrocycles were evaluated as discrete molecular catalysts, interface-anchored composites, and extended organic polymers[1], enabling direct comparison of active-site identity, charge transport[2], and stability under electrocatalytic conditions[3,4].

Metal-free porphyrin and phthalocyanine systems demonstrate that the nitrogen-rich macrocyclic core can serve as an intrinsic active site for proton reduction and water oxidation, with catalytic activity strongly modulated by meso-substituent electronics and linker identity.[1] Electron-withdrawing substituents tune imine basicity and dictate mechanistic pathways for hydrogen evolution, transitioning between proton-first and electron-first sequences, as supported by electrochemical analysis, foot-of-wave kinetics, and density functional theory.[2] In polymeric architectures, condensation-derived porphyrin and phthalocyanine networks exhibit enhanced conductivity, mass transport, and operational stability relative to their molecular counterparts.[3]

Metal incorporation introduces complementary catalytic behavior. Cobalt and iron porphyrin polymers display bifunctional activity toward the hydrogen and oxygen evolution reactions across acidic and basic media, while interface anchoring of cobalt porphyrins onto conductive hexahydroxytriphenylene-based metal–organic frameworks decouples catalytic turnover from charge transport limitations. In these composites, the macrocyclic metal center remains the electroactive site, whereas the extended framework facilitates electron transfer and interfacial adsorption processes. These studies highlight how molecular-level electronic tuning, metal coordination, and framework integration control catalytic performance in macrocyclic electrocatalysts, offering design principles for energy-relevant water splitting systems based on porphyrins and phthalocyanines.

REFERENCES

1. "Metal-Free Phthalocyanine-Based Polymer for Bifunctional Electrochemical Water Splitting" Alexandria Castillo, Neidy Ocuane, Jacqueline Guzman James, Jorge Gardea-Torresdey, and Dino Villagrán ACS Electrochemistry Article ASAP DOI: 10.1021/acselectrochem.5c00435

2. "Mechanistic Study on the Electronic Tuning of Metal-Free Porphyrins for Hydrogen Evolution Reaction" Yulu Ge, R. Rebeca Favela Robledo, Jonathan J. Calvillo Solis, Anthony Denning, Neidy Ocuane, Dino Villagrán, *ACS Electrochemistry,* **2025** ASAP, https://pubs.acs.org/doi/10.1021/acselectrochem.5c00259

3. "Metalloporphyrin organic polymers as effective and stable electrocatalysts for the oxygen and hydrogen evolution reactions" Yulu Ge, Neidy Ocuane, Anthony Denning, Yanyu Wu, Joel Sanchez, Mario V Ramos-Garcés, Jorge L Colón, Thomas F Jaramillo, Dino Villagrán, *Molecular Catalysis*, **2025**, 115483 https://doi.org/10.1016/j.mcat.2025.115483

4. Interface Anchoring of Cobalt Porphyrin on a Conductive Metal Organic Framework Platform for Water Electrolysis[Neidy Ocuane, Brooke A. Dorsey, Satya Prakash Suman, Marco Ramírez Ramos, Harish Banda, and Dino Villagrán, *ACS Applied Materials & Interfaces* **2026** 18 (1), 1312-1323 DOI: 10.1021/acsami.5c19333

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Zn Dipyrrins: Exciton Coupling, Excitation Energy Dynamics and Applications in Biosensing

Luca Ravotto,[a,b] Mirna El Khatib,[a,b] Dabin Kim,[b,c] April Bialas,[d] Thomas Troxler,[a,b] Simin Belali,[a,b] Andrei V. Cheprakov,[d] Frank Spano,[e] Jessica M. Anna,[b,c] Sergei A. Vinogradov,[a,b]

[a] *Department of Biochemistry and Biophysics, University of Pennsylvania, Philadelphia, USA*
[b] *Department of Chemistry, University of Pennsylvania, Philadelphia, USA*
[c] *Department of Chemistry, University of Pittsburgh, Pittsburg, USA*
[d] *Department of Chemistry, Moscow State University, Moscow, Russia*
[e] *Department of Chemistry, Temple University, Philadelphia, USA*

Dipyrrins form a versatile class of dyes with applications ranging from light harvesting to biomedical imaging. The mode of the central ion coordination and the ensuing molecular geometry play a key role in the photophysics of metal complexes of dipyrrins. We used a range of spectroscopic and computational methods to investigate the excited state dynamics of Zn(II) complexes of *meso*-aryl-dipyrrins containing ester groups in 2,2'-positions. In solutions in the presence of Zn^{2+}, dipyrrin-2,2'-diesters exist as mixtures of *mono*- (LZnX) and *bis*- (L_2Zn) complexes. LZnX complexes are strongly fluorescent, while in L_2Zn, the dipyrrin ligands are oriented in non-orthogonal fashion, resulting in strong exciton coupling and fluorescence quenching. The presence of exciton coupling in L_2Zn was confirmed by two-dimensional electronic spectroscopy (2DES) in combination with spectral modeling and DFT/TDDFT calculations. The evolution of the initially populated Frenkel excitonic states appears to involve an intermediate state possibly having a charge transfer character. These results have major implications for the design of dipyrrin-based sensors of Zn^{2+}. The apparent dissociation constants of Zn complexes of water-soluble dipyrrin-2,2'-diesters and dipyrrin-2,2'-diamides (K_d's) were originally reported to be in the 10-100 μM range; however, the above spectroscopic investigation revealed that the measured constants could have been related not to binding of Zn^{2+} by free-base dipyrrins, but rather to dissociation of non-fluorescent L_2Zn in the presence of excess Zn^{2+}. Detailed spectroscopic titrations confirmed this conjecture, suggesting, in turn, that the actual K_d's for Zn binding by dipyrrins are in nM/low-μM range. Taken together, these measurements provide new information about photophysics of dipyrrins and offer useful clues for the future design of dipyrrin-based sensors for biological applications.

REFERENCES

1. Filatov, M. A.; Lebedev, A. Y.; Mukhin, S. N.; Vinogradov, S. A.; Cheprakov, A. V. *J. Am. Chem. Soc.* **2010,** *132* (28), 9552-9554.
2. Thyagarajan, S.; Ghosh, B.; Filatov, M. A.; Moore, A. V.; Cheprakov, A. V.; Vinogradov, S. A. *SPIE BiOS* **2011,** *7910*, DOI: 10.1117/12.873654.
3. El Khatib, M.; Cheprakov, A. V.; Vinogradov, S. A. *Inorg. Chem.* **2022,** *61* (32), 12746-12758..
4. Kim, D.; Ravotto, L.; Bialas, A.; Troxler, T.; Ou, Z. P.; Kadish, K. M.; Cheprakov, A. V.; Spano, F. C.; Vinogradov, S. A.; Anna, J. M. *J. Phys. Chem. B* **2025,** *129* (39), 10049-10062.

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Pd(II) Porphyrin-UCNP Hybrid Biocompatible Systems: Design and Structural Features

M. V. Volostnykh,[a] P. A. Demina,[a,b] K. V. Khaydukov,[a] E. V. Ermakova,[a] A. O. Dushina,[a] R. A. Akasov[b] and Y. G. Gorbunova[a,c]

[a] *Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Moscow*
[b] *Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Moscow*
[c] *Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow*

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Determination of dissolved molecular oxygen (DO) in biological media is a crucial task in modern medical diagnostics. Optical sensors, particularly in their miniature forms, are the most suitable for real-time quantitative DO measurements in cells and tissues of living organisms.

Pd(II) porphyrinates are efficient oxygen-sensitive phosphors; however, their UV/Vis excitation limits their applicability for deep-tissue imaging. To overcome this limitation, we developed strategies to combine them with core/shell upconversion nanoparticles (**UCNP**s: $NaYF_4$:Yb^{3+},Er^{3+}@$NaYF_4$ and $NaYF_4$:Yb^{3+},Tm^{3+}@$NaYF_4$), which convert NIR excitation (975 nm) into visible emission within the "tissue transparency window" (650–1300 nm).

A series of hydrophobic and water-soluble Pd(II) porphyrinates (**PdPor**) were synthesized for use as oxygen-sensitive acceptors in hybrid systems, using both established [1] and newly developed [2] methods. Their aggregation behavior [2] and biochemical properties (BSA binding, cytotoxicity, cellular uptake) were then investigated in detail, as these factors can significantly affect their luminescence. Crystallographic analysis revealed that upon moving from tetra- to disubstituted Pd(II) complexes, π–π stacking interactions become more pronounced, leading to the assembly of "head-to-tail" supramolecular porphyrin chains. As a result, the series was restricted to tetrasubstituted derivatives, including benzoporphyrins, with different functional groups. The water-soluble tetrasubstituted **PdPor** bearing monoethylphosphonate groups was found to be generally non-cytotoxic toward mouse cell lines, except for enhanced toxicity toward RAW 264.1 macrophages at 40 μM. Moreover, it was non-toxic to cancer cells (4T1) and fibroblasts (L929), where it even slightly improved cell viability. Notably, it also showed the highest cellular accumulation in MCF-7 human breast carcinoma cells, which was influenced by the presence of proteins in the medium.

NIR-absorbing donor **UCNP**s were obtained by thermal decomposition of the corresponding trifluoroacetates CF_3COOX (X = Na, Y, Yb, Er, Tm) and functionalized with biocompatible polymers (polyethylenimine, maleic anhydride copolymer, SiO_2), thus providing good colloidal stability (over 14 days).

The principal possibility of FRET in **PdPor**–**UCNP** hydrophobic nanocomplexes — obtained by mixing the components in chloroform — was demonstrated, with energy transfer efficiencies of 33% (410 nm) and 17% (520 nm).

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REFERENCES

1. M.V. Volostnykh, S.M. Borisov, M.A. Konovalov, A.A. Sinelshchikova, Y.G. Gorbunova, A.Y. Tsivadze, M. Meyer, C. Stern, A. Bessmertnykh-Lemeune, *Dalton Trans.* **2019**, 48, 8882–8898.
2. M.V. Volostnykh, G.A. Kirakosyan, A.A. Sinelshchikova, E.V. Ermakova, Y.G. Gorbunova, A.Y. Tsivadze, S.M. Borisov, M. Meyer, L. Khrouz, C. Monnereau, S. Parola, A. Bessmertnykh-Lemeune, *Dalton Trans.* **2025**, 54, 2340-2356.

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Using Molecular (Porphyrin) Rings to Functionalize Carbon Allotropes and Create Few-Qubit Architectures

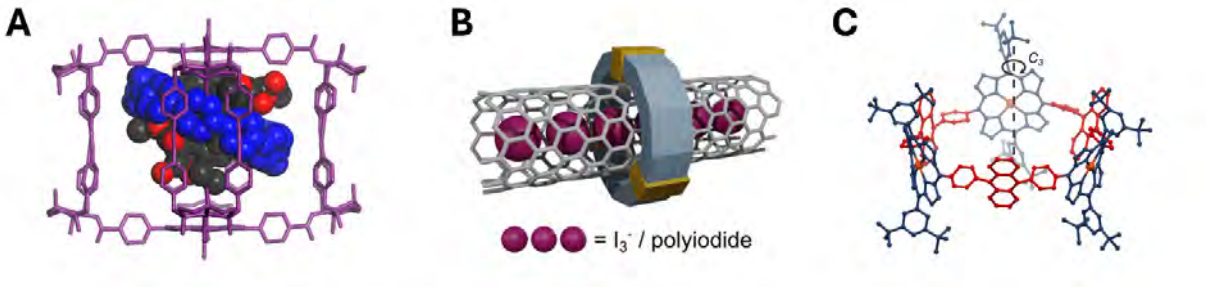
Max von Delius[a]

[a] *Institute of Organic Chemistry, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany*

Molecular rings ("macrocycles" or "hosts") have long been used by chemists to encapsulate ions or molecules ("guests"). Over the past two decades, curved rings have bind used to bind, solubilize and functionalize curved carbon allotropes (fullerenes, SWCNTs).[1]

In this talk, I will present recent work by our group on three challenges that will be of interest to the ICPP community (prophyrins, fullerenes, SWCNTs, spintronics, quantum sensing):

A) Can **Zn-porphyrin** cages and π-curved macrocycles be used to control the selectivity of **fullerene** (multiple-)addition reactions?[2]
B) Can rigid rings be used to functionalize and disperse **SWCNTs** in water?[3]
C) Can rigid **Cu-porphyrin** rings be used to precisely control the relative geometry and orientation of **molecular qubit candidates** and endow them with unusual optical and magnetic properties?[4]



REFERENCES

1. (a) Y. Xu, M. von Delius, *Angew. Chem. Int. Ed.* **2020**, *59*, 559; (b) X. Chang, Y. Xu, M. von Delius, *Chem. Soc. Rev.* **2024**, *53*, 47–83.
2. (a) Y E. Ubasart, O. Borodin, M. von Delius, X. Ribas et al. *Nat. Chem.* **2021**, *13*, 420; (b) F. Steudel, G. Pavan, X. Ribas, M. von Delius et al. *Angew. Chem. Int. Ed.* **2023**, *62*, e202309393; (c) F. Schwer, S. Zank, M. Freiberger, F. M. Steudel, N. Geue, L. Ye, P. E. Barran, T. Drewello, D. M. Guldi, M. von Delius *Angew. Chem. Int. Ed.* **2024**, *63*, e202413404.
3. J. Kraus, L. Meingast, U. Kaiser, J. Maultzsch, M. von Delius et al. *Angew. Chem. Int. Ed.* **2024**, *63,* e202402417.
4. X. Chang, A. Redman, L. Zedler, B. Dietzek-Ivanšić, S. Richert, M. von Delius et al., *Angew. Chem. Int. Ed.* **2025**, *64*, e22950.

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What Dipoles Have to Do with Anything?

Val I. Vullev[a]

[a]*University of Calieofnia, Riverside, CA 92507, USA.*

Charge transfer (CT) sustains life on earth and ensures our modern ways of leaving possible [1]. CT is at the centre of photosynthesis, and understanding how to control it and improve the efficiency of the desired processes is crucial for energy sustainability. Dipoles are ubiquitous, and their effects on CT are enormous [2]. We undertake bioinspired approaches that offer key paradigms for advancing artificial photosynthesis [3]. We design and devlop bioinspired molecular electrets, comprising anthranilamide (AA) residues, to explore emerging dipole effects on CT [3]. Even a single electret residue can rectify CT and exert enormous effects on CT kinetics [2,4]. As commonly accepted, dipoles affect CT thermodynamics, which alters the Franck-Condon contributions to the rate consents. Conversely, we discovered that the dipoles can also strongly affect the donor-acceptor electronic coupling, turning the accepted paradigms upside down. Going beyond the static models, we discovered that the macrodipoles of the AA molecular electrets are highly dynamic and exhibit picosecond fluctuations with amplitudes that can vary between 50% and 200% of their average values [5]. Our analysis reveals that these fluctuations originate from the solvent dynamics around the solvation cavity of the electrets, i.e., from transient short-lived alignments of the solvent dipoles inducing fluctuations in the Onsager reaction field. Extending our studies reveals that this phenomenon is universal, emerging even for solvated nonpolar molecules. It presents paradigm-shifting ways of thinking about electrostatic interactions in condensed media and how they affect energy conversion, information flow, and the overall performance of electrinc materials and devices.

REFERENCES

1. *Phys. Chem. Chem. Phys.* **2020**, *22*, 21583–21629.
2. *Angew. Chem. Int. Ed.* **2018**, *57*, 12365-12369.
3. *J. Phys. Chem. Lett.* **2011**, *2*, 503-508.
4. *J. Am. Chem. Soc.* **2014**, *136*, 12966-12973.
5. *J. Am. Chem. Soc.* **2024**, *146*, 5162-5172.

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Porphycenes: experimental and theoretical studies of photophysics, photostability, and single molecule detectability

A. Listkowski,[a,b] A. Gajewska,[a] M. Kijak,[a] I. Mbakara,[a] A. Jamrozik,[a] A. Gorski,[a] B. Golec,[a,b] J. Waluk[a]

[a] *Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland*
[b] *Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University, 01-815 Warsaw, Poland, Dewajtis 5, 01-815 Warsaw, Poland*

Our studies of porphycenes combine syntheses with detailed spectral and photophysical characterization. Recently obtained families of porphycenes bear single or multiple alkyl/aryl/nitro/amino/halogen functionalities or their combinations located at topologically different positions of the macrocylcle skeleton. Emission intensities and lifetimes of these compounds vary dramatically, depending on the number and position of substituents. Differences in fluorescence quantum yields reach three orders of magnitude in routinely used solvents, but become much smaller when the fluorophore is placed in a rigid environment. Based on quantum chemical calculations, we propose a model that is able to explain these differences in photophysics.

Given a vast applicational potential of porphycenes in areas exploiting interaction with light, it is crucial to find ways of maximizing their photostability. We demonstrate how the quantum yield of photobleaching can be decreased (or enhanced) via specific, position-dependent substitution. An important observation is the drastic change in photostability while replacing electron-donating substituents with electron-withdrawing ones. We also point out that a reliable prediction of resistance to photodegradation must include both static, electronic factors (redox potentials) and kinetic photophysical parameters (efficiency of formation and lifetime of the triplet state).

Porphycene is one of a few molecules that have been observed on a single molecule level using three different techniques: (i) confocal fluorescence and (ii) Raman microscopy, as well as (iii) scanning probe microscopy. The fact that single porphycene molecules can be detected by fluorescence could look surprising, because of efficient population of the triplet state. We have proven [1] that, under conditions of measurements – low concentration of fluorophore embedded in a polymer matrix – only a subpopulation of the chromophore is observed, consisting of molecules that have a triplet quencher (molecular oxygen) in their vicinity. This conclusion, which seems quite general for most of aromatic molecules, has been confirmed by spectroscopic and photophysical studies of porphycene embedded in rare gas or nitrogen cryogenic matrices to which a controlled amount of oxygen was being added.

REFERENCES

1. A. Jamrozik, A. Gorski, B. Golec, J. Waluk, *J. Phys. Chem. C* **2025**, *129*, 22435-22442;
DOI: 10.1021/acs.jpcc.5c05272

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Covalent Organic Frameworks Based on pi-Extended Porphyrins: Synthesis and Characterization

Ting Han, Nikhil Kumar, Kendra Hamilton, Yuanxi Wang, Jens Neu, Saad Shiakh, Hong Wang

Department of Chemistry, University of North Texas, Denton, TX 76201, USA

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Covalent organic frameworks (COFs) represent an exciting and fast-growing field in materials science.[1, 2] 2D COFs containing aromatic units can form vertically aligned *pi*-columns, which can induce interlayer electronic communication along the *pi*-stacking direction. pi-Electronic COFs have shown semiconductor characteristics and have demonstrated potentials as charge-carrier transporters, light emitters, photoconductors, light-harvesting antennae, and photoenergy-converting materials. Porphyrins are known to possess exceptionally rich electronic and photophysical properties. The photoexcited kinetics and dynamics of porphyrins play a key role in determining the functions of porphyrins in their applications. The incorporation of porphyrins into COFs will provide photonic and electronic materials, opening broad opportunities to enable extensive applications of COFs in energy conversion and storage.[3-5]

In this presentation, the synthesis and characterization of new class of 2D COFs including donor-acceptor (D-A) COFs and fully cyclically conjugated COFs will be presented. The suitability of the pi-extended porphyrin monomer as building blocks for COFs has been investigated and analyzed. The formation of the D-A COFs was verified by several characterization techniques including Powder X-ray diffraction (PXRD), Fourier-transform infrared (FT-IR) spectra, solid state ^{13}C NMR spectroscopy and scanning electron microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS). Solid UV-Vis absorption spectroscopy has revealed band gaps of 1.54 - 1.63 eV for these COFs, suggesting their semiconducting nature. Temperature resolved THz-transmission measurements were used to measure the optical conductivity of the ground state. The D-A COFs exhibits high conductivity of approximately of 1 S/m - 2 S/m (at 1THz). The preliminary calculations for these COFs revealed a donor-acceptor character, where conduction band edge states are localized on the dibenzoporphyrin linkers (yellow) and valence band edge states at TAPP cores (grey). This donor-acceptor character likely contributes to their high optical conductivity.

REFERENCES

1. D. Jiang, V. G. W. Tan, Y. Gong, H. Shao, X. Mu, Z. Luo and S. He, *Chem. Rev.*, 2025, **125**, 6203-6308.
2. N. Keller and T. Bein, *Chem. Soc. Rev.*, 2021, **50**, 1813-1845.
3. J. Yin, L. Sang and Y. Wang, *Nanomaterials (Basel)*, 2025, **15**.
4. T. Sun, Z. Wang, Y. Wang, Q. Xu, K. Wang and J. Jiang, *Angew. Chem. Int. Ed.*, 2025, **64**, e202422814.
5. X. G. Li, J. Li, J. Chen, L. Rao, L. Zheng, F. Yu, Y. Tang, J. Zheng and J. Ma, *Biomater. Sci.*, 2024, **12**, 2766-2785.

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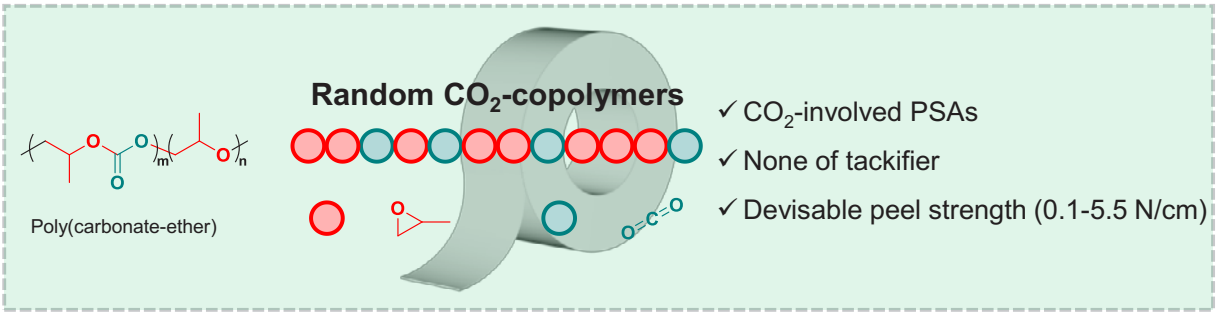
Sustainable Pressure-Sensitive Adhesives Derived from CO_2-Based Polymers

Xianhong Wang[a,b], **Shunjie Liu**[a,b]

[a]*State Key Laboratory of Polymer Science and Technology, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences; No.5625, Renmin Street, Changchun, Jilin, 130022, P. R. China*
[b]*School of Applied Chemistry and Engineering, University of Science and Technology of China; No.96, JinZhai Road, Hefei, Anhui, 230026, P. R. China*
E-mail: xhwang@ciac.ac.cn, sjliu@ciac.ac.cn,

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Pressure-sensitive adhesives (PSAs) are materials that quickly adhere to substrates with minimal pressure. However, most commercial PSA formulations still rely on non-biodegradable polymers such as polyacrylate derivatives, rubbers, and silicones. In response to increasing environmental concerns, eco-friendly PSAs have become the fastest-growing segment in this technology. In this study, we present a sustainable approach to developing PSAs through the random copolymerization of CO_2 and propylene oxide, catalyzed by a polymeric porphyrin aluminum complex.[1, 2] The use of this polymeric porphyrin catalyst, combined with the immortal polymerization method, allows precise control over the copolymer structure and enables the tailored design of the polymer's chain segment composition. The resulting CO_2-based polymers, featuring rigid carbonate units and flexible ether units, exhibit excellent viscoelastic properties. These properties not only outperform those of conventional adhesives without the need for tackifiers but also highlight the simplicity and efficiency of the synthesis process.



REFERENCES

1. Z. Zhou, X. Wang, S. Liu, T. Lang, S. Cheng, X. Pang, X. Chen, X. Wang, ChemSusChem 2025, 18, e202402546.
2. Z. Zhou, S. Liu, L. Yang, Q. Kuang, H. Zhou, C. Zhuo, X. Wang, ACS Catal. 2023, 13, 15116.

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Mechanisms of ligand-dependent activation of bacterial globin coupled sensors

Emily E. Weinert[a]

[a]*Department of Biochemistry and Molecular Biology, Penn State University, University Park, PA 16802 USA*

Heme proteins have evolved to carry out a diverse array of functions, from oxidative chemistry to O_2 transport. In addition, multiple families of heme proteins serve as bacterial gas sensors, controlling metabolism, growth, and biofilm formation. Globin coupled sensors (GCSs) are bacterial heme proteins that consist of a globin domain linked by a central domain to an output domain, such as diguanylate cyclase domains that synthesize c-di-GMP, a major regulator of biofilm formation and virulence. Comparison of different GCS proteins has identified heme pocket residues involved in modulating O_2 affinity, as well as ligand-dependent activation of GCS proteins. Using equilibrium oxygen binding studies, we have demonstrated that a subset of GCS proteins bind oxygen cooperatively and have identified residues required for allosteric communication between hemes. Building on these results, we are using a combination of resonance Raman spectroscopy, hydrogen-deuterium exchange mass spectrometry, and enzyme assays to investigate the mechanism by which ligand binding at the heme controls protein dynamics and conformational changes to yield ligand-dependent regulation of cyclase domain activity. Taken together, these studies provide new insights into the mechanism by which ligand binding modulates heme-protein interactions to control activity and downstream signaling of GCSs, as well as the broader physiological effects of O_2 sensing, including bacterial growth and virulence.

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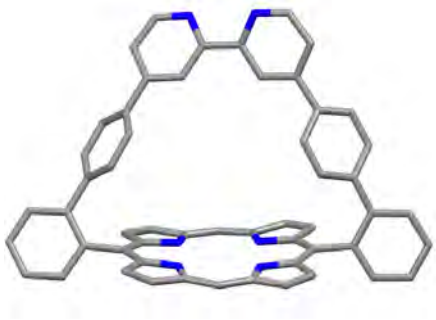


A 35 year journey in strapped porphyrin self-assembly

Jean Weiss

Institut de Chimie de Strasbourg, CNRS-Université de Strasbourg, France

Over the last 35 years, diimine strapped porphyrins have been developed in our group and have proven extremely versatile as far as their applications are concerned.[1] In this presentation, findings that led to linear objects by self-assembly will be recalled and recent synthetic developments leading to a new class of inverted strapped porphyrins that are candidates for 3D organized multichromophores will be presented.



REFERENCES

1. Light triggers molecular shuttling in rotaxanes: control over proximity and charge recombination. M. Wolf, A. Ogawa, M. Bechtold, M. Vonesch, J. A. Wytko, K. Oohora, S. Campidelli, T. Hayashi, D. M. Guldi, J. Weiss *Chem. Sci.* **2019**, *10*, 3846-3853.
2. Controlled growth of porphyrin wires at a solid-liquid interface. C. Kahlfuss, Y. Kikkawa, J. A. Wytko, J. Weiss *Helv. Chim. Acta*. **2019**, *102*, e1900058.
3. Metal-mediated linear self-assembly of porphyrins. J. A. Wytko, R. Ruppert, C. Jeandon and J. Weiss, *Chem. Commun*., **2018**, *54*, 1550-1558.

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Modeling Heme Peroxo Chemistries that Drive Biologically and Synthetically Crucial Transformations

Gayan Wijeratne*[a], Shanuk Rajapakse[a], Dhilanka Udukalage[a], and Steven Zheng[a]

[a]*Department of Chemistry & Biochemistry, University of Alabama, Tuscalosa, AL 35401.*

Heme enzymes mediate a variety of paramount oxidation and oxygenation reactions in a wide variety of organisms including humans, and thus have been implicated in many important disease situations. Hence, meticulously designed synthetic model compounds of such systems can be of prime importance, mainly since they can be powerful mechanistic probes for understanding many of the biologically relevant mechanistic ambiguities. Oxygen activating heme enzymes have been known for nearly a century, nonetheless, a rigorous mechanistic understanding is far from complete. In particular, reaction pathways driven by mid-valent intermediates such as heme superoxo, peroxo, hydroperoxo, species have proven to be challenging to comprehend given the significant versatility in their structural and functional attributes. Heme peroxo intermediates represent an important branching point in a multitude of these reaction landscapes, mediating a rich collection of organic substrate interconversions with far-reaching effects within (human and other) physiological systems. How precisely are their geometric and electronic structures are fine-tuned to efficiently carry out the multifaceted reactivities is not very well understood, wherein important parameters pertaining to their primary and secondary coordination spheres play key roles. Particularly, distinct structural properties that govern the remarkable variety of reactivity profiles of heme peroxo intermediates will be discussed in detail, drawing examples from both biologically and synthetically relevant transformations.

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Bimetallic porphyrin PET radiotracers for Low-Dose MRI contrast enhancement

Ka-Leung Wong

[a]*Department of Chemistry, City University of Hong Kong, Hong Kong SAR, China*

Concerns about the risks posed by medical imaging agents have prompted ongoing efforts to develop safer and more efficient compounds. Among these, dual-modal imaging strategies combining positron emission tomography (PET) and magnetic resonance imaging (MRI) remain highly desirable, yet no single-molecule probe has previously achieved this without performance compromise. We herein present **PGaLGd**, a bimetallic single-molecule imaging agent that incorporates radioactive ^{68}Ga(III) as a PET radiotracer and coordinated Gd(III) for MRI contrast. This design enables simultaneous PET/MRI dual imaging at low concentrations, with the non-radioactive precursor exhibiting inherently high T1-relaxivity both before and after microwave-assisted radiolabeling, thereby reducing the overall dosage required. Computational chemistry studies elucidated the MRI-enhancing mechanisms, highlighting the importance of interlinked structures, coordinated metals, adjacent ligands, and frontier molecular orbitals in optimizing water relaxation ability. *In vivo* imaging in mice confirmed the dual-modality performance, while comprehensive *in vitro* and *in vivo* evaluations demonstrated favorable biosafety and substantial photodynamic therapeutic effects across cell lines, organoids, and animal models. Together, these findings establish **PGaLGd** as a promising next-generation low-dose imaging agent with integrated diagnostic and therapeutic potential.

ORALS

REFERENCES

1. Yue Wu, Yuen-Ting Wong, Yik-Hoi Yeung, Pak-Lun Lam, Ho-Fai Chau, Wing-Sze Tam, Qian Zhang, William C. S. Tai* and Ka-Leung Wong*, 'Peptide Multifunctionalization via Modular Construction of trans-AB$_2$C Porphyrin on Resin', *Advanced Science,* (2025) 2409771.
2. Chen Xie, Xiong Li, Leilei Zhang, Ho-Fai Chau, Waygen Thor, Wing Sze Tam, Benjamin Woolley, Mingjun Jiang, Chi-Fai Ng, Mauro Botta, Tao Zhang*, Nicholas J. Long*, Ga-Lai Law* and Ka-Leung Wong*, 'Bimetallic porphyrin PET radiotracers for low-dose MRI contrast enhancement'*, Chemical Engineering Journal*, (2024) 495, 153350
3. Y. Wu, H.-F. Chau, Y.-H. Yeung, W. Thor, H.-Y. Kai, W.-L. Chan* and K.-L. Wong*,'Versatile synthesis of multivalent porphyrin–peptide conjugates by direct porphyrin construction on resin', *Angewandte Chemie International Edition*, (2022) e202207532.

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Stable Corrole Radicals: Spectroscopic Features and Photo-Functional Modulation

Fan Wu[a,b], Hu Gao[b,c], Pengfei Li[b], and Zhen Shen[b]

[a] *School of Chemistry and Materials Science, Nanjing Normal University, Nanjing, 210023*
[b] *School of Chemistry, Nanjing University, Nanjing 210023, China*
[c] *College of Materials Science and Engineering, Nanjing Forestry University, Nanjing 210037, China*

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Organic radicals hold great promise for molecular spintronics and phototherapeutics owing to their intrinsic magnetic moments, efficient redox activity, and unique photophysical behaviors. However, their susceptibility to degradation under operational conditions poses a fundamental challenge for practical applications. Porphyrinoids have emerged as an ideal radical platform via spin delocalization across their π-conjugated frameworks. Corroles are contracted analogues of porphyrins. Unlike typical porphyrins, which are Hückel-aromatic with [4n+2]π electrons, corroles possess a trianionic core and a reduced N4 cavity. These features facilitate unique metal-coordination chemistry and the formation of [4n+1]π radical species [1]. We construct a series of highly stable radical complexes by fusing cycloalkyl or aromatic groups at the β-pyrrolic positions of corroles, enabling effective modulation of their redox and photophysical properties [2-6]. By combining experimental results with theoretical analysis, we elucidated the relationship between the absorption spectral changes of these radicals at different oxidation states and their aromaticity. The resulting radicals exhibit reversible aromatic-to-antiaromatic switching and broad absorption bands extending to the near-infrared region, showing intriguing performance as photothermal agents in phototheranostic applications.

REFERENCES

1. Gao, H.; Wu, F.; Wang, K.; Shen, Z., Recent developments in corrole radicals. J. Porphyr. Phthalocyanines 2023, 27 (07n10), 946-957.
2. Gao, H.; Wu, F.; Zhao, Y.; Zhi, X.; Sun, Y.; Shen, Z., Highly Stable Neutral Corrole Radical: Amphoteric Aromatic–Antiaromatic Switching and Efficient Photothermal Conversion. J. Am. Chem. Soc. 2022, 144 (8), 3458-3467.
3. Gao, H.; Wu, F.; Zhao, Y.; Yang, X.; Shen, Z., Redox-switchable bistable nickel corrole. Inorg. Chem. Front. 2023, 10 (10), 3037-3046.
4. Gao, H.; Zhi, X.; Wu, F.; Zhao, Y.; Cai, F.; Li, P.; Shen, Z., Molecular Engineering of Corrole Radicals by Polycyclic Aromatic Fusion: Towards Open-Shell Near-Infrared Materials for Efficient Photothermal Therapy. Angew. Chem. Int. Ed. 2023, 62 (40), e202309208.
5. Wu, F.; Gao, H.; Zhao, Y.; Shen, Z., Ground state singlet-to-triplet conversion of copper corrole radical by β-benzo-fusion. Chin. Chem. Lett. 2023, 34 (8), 107994.
6. Li, P.; Qu, C.; Wu, F.; Gao, H.; Zhao, C.; Zhao, Y.; Shen, Z., Robust free-base and metalated corrole radicals with reduction-induced emission. Chin. Chem. Lett. 2025, 36 (2), 110292.

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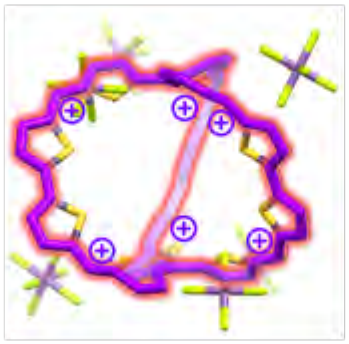


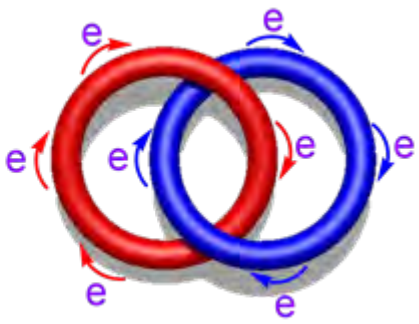
Porphyrinoid Based Molecular Cages and [2]Catenanes

Jishan Wu[a]

[a]*Department of Chemistry, National University of Singapore, 3 Science Drive 3, 117543, Singapore*

This lecture will primarily delve into the synthesis, electronic properties, and aromaticity of pophyrinoid-based, 3D fully π-conjugated molecular cages and mechanically interlocked molecules. Notably, three-dimensional global aromaticity has been achieved in thiophene-based molecular cages.[1] This phenomenon can be elucidated by the two-dimensional Hückel/Baird aromaticity observed in the individual constitutional macrocycles in their respective singlet or triplet states. We also observed unique through-space electronic coupling between two globally (anti)aromatic rings in a catenane structure.[2]





REFERENCES (05_REFERENCES_TITLE)

1. (a) Y. Ni, T. Y. Gopalakrishna, H. Phan, T. Kim, T. Herng, Y. Han, T. Tao, J. Ding, D. Kim, J. Wu, *Nat. Chem.* **2020**, *12*, 242. (b) L. Ren, Y. Han, X. Hou, Y. Ni, J. Wu, *Chem* **2021**, *7*, 3442. (c) S. Wu, Y. Ni, Y. Han, X. Hou, C. Wang, W. Hu, J. Wu, *Angew. Chem. Int. Ed.* **2022**, *61*, e202115571. (d) S. Wu, Y. Ni, Y. Han, S. Xin, X. Hou, J. Zhu, Z. Li, J. Wu, *J. Am. Chem. Soc.* **2022**, *144*, 23158.
2. Y. Sui, J. Hao, S. Wu, L. Ren, Z. Zeng, J. Wu, Y. Ni, *Nat. Synth.* **2025**, DOI: 10.1038/s44160-025-00918-0

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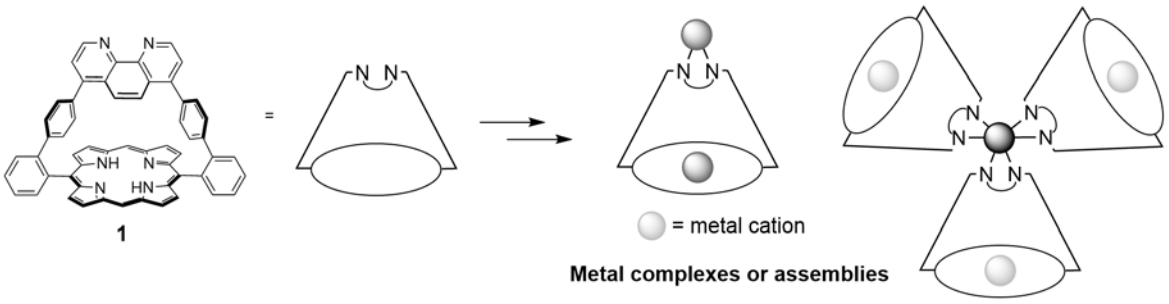
Multi-metallic complexes and assemblies built from a strapped-porphyrin

Jennifer Wytko[a], Léa Depret[a], and Jean Weiss[a]

[a]*Institut de Chimie de Strasbourg, UMR 7177, CNRS-Université de Strasbourg, Strasbourg, France*

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Over many years, our phenanthroline-strapped porphyrin has demonstrated multiple uses, from hemeprotein models to building blocks for self-assembled dyads and multi-porphyrin wires [1]. Now, the phenanthroline subunit has been oriented with the nitrogen atoms towards the outside of the strap in porphyrin **1** (see figure below) to explore its coordination chemistry and the properties of multi-metallic assemblies. Homo-bimetallic lanthanide complexes are of interest for cooperative upconversion [2], whereas hetero-bimetallic metal complexes or multi-porphyrin assemblies are potential antenna-like systems for electron or energy transfer [3]. Synthetic strategies, coordination chemistry and, possibly, initial fluorescence studies will be presented.



REFERENCES

1. C. Kahlfuss, J. A. Wytko, J. Weiss, *ChemPlusChem*, **2017**, *82*, 584; b) M. Hananaa, C. Kahlfuss, J. Weiss, R. Cornut, B. Jousselme, J. A. Wytko, S. Campidelli, *C. R. Chimie* **2021**, (3) 1.
2. L. Charbonnière, A. M. Nonat, R. C. Knighton, L. Godec, *Chem. Sci*. **2024**, *15*, 3048.
3. G. Santosh, *Asian J. Chem*. **2018**, *30*, 1836.

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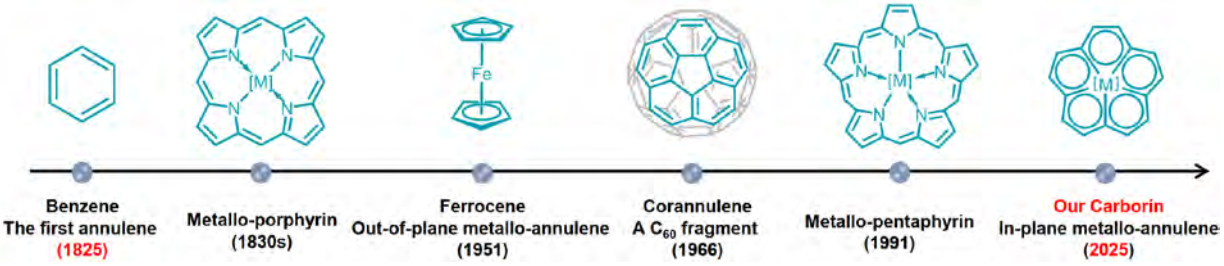


Metal-Centered Planar [15]Annulenes

Haiping Xia

Shenzhen Grubbs Institute and Guangdong Provincial Key Laboratory of Catalysis, Department of Chemistry, Southern University of Science and Technology, Shenzhen 518055, China

Out-of-plane metallo-annulenes, such as ferrocene, have played a widespread role in both fundamental research and technology since their discovery in the 1950s. In stark contrast, the integration of metal within the annulene core to achieve in-plane metallo-annulenes, has been obstructed not only by the synthetic trouble and the non-planarity of annulenes with appropriate internal dimensions, but also by the difficulty of embedding the metal. Here, we present the preparation and characterization of the first in-plane metallo-annulene framework, a D_{5h} symmetric metal-centered [15]annulene in which the metal center is shared by five identical five-membered rings.[1] This structure may be viewed as a planarized architecture obtained formally by replacing the inner five-membered ring of corannulene (a C_{60} fragment) with a transition metal center. It also represents an expanded, all-carbon analogue of a metallo-porphyrin (metallo-pentaphyrin), thus bridging annulene chemistry and porphyrin chemistry. We proposed the term "**carborin**", derived from a combination of three words: ***carbo***long (a key precursor), ***rin***g (to emphasize the macrocyclic nature) and porphy***rin*** (to underscore the metal coordination), to describe this new class of annulene.[2] Theoretical analyses reveal the unique nature of its aromaticity: not only does the [15]annulene possess global aromaticity, but the five-membered metallacycles also exhibit local aromaticity. Consequently, the central metal is shared by 5 aromatic rings, which represents a world record for any transition metal. Due to its strong aromaticity, the present system display high stability. Furthermore, it can be modified easily in a post-synthetic fashion, not only in the annulene plane, but also in the axial direction. These attributes underscore its potential as a versatile and promising building block for materials science. It is worth noting that the first discovered annulene is benzene reported by Faraday in 1825,[3] therefore, our carborin could be used to commemorate the bicentennial of the discovery of benzene.



REFERENCES

1. Xu, B. ; Chen, D. ; Ruan, K. ; Luo, M. ; Cai, Y. ; Qiu, J. ; Zhou, W. ; Cao, B. ; Lin, Z. ; Sessler, J. L. ; Xia, H. Metal-centred planar [15]annulenes. *Nature* **2025**, *641*, 106.
2. Xu, B. ; Chen, D. ; Xia, H. A journey from carbolong complexes to in-plane metallo-annulenes. *Chem* **2025**, *11*, 102786.
3. Faraday, M. On new compounds of carbon and hydrogen, and on certain other products obtained during the decompostion of oil by heat. *Philos. Trans. R. Soc. London.* **1825,** *115*, 440.

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Porphyinoid monomers and dimers with tunable aromaticity based on the N-confusion approach

Qizhao Li, Yanping Huang, Guangxian Su, Yongshu Xie

Key Lab for Advanced Materials, East China University of Science & Technology, 200237, Shanghai, China.

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Porphyrinoids have attracted considerable attention because of their distinctive properties that can be employed for applications in various areas [1]. One important research topic in the area of porphyrin chemistry is aromaticity, and various porphyrinoids have been reported to achieve tunable aromaticity [2]. In this respect, we have reported various porphyrinoids with tunable aromaticity by oxidatively linking the two terminal pyrroles of pentapyrrins and hexapyrrins [3]. We have also employed the so-called "Confusion" approach [4] to develop porphyrinoid dimers with tunable aromaticity by incoporating α-β-linked pyrrole units [5].

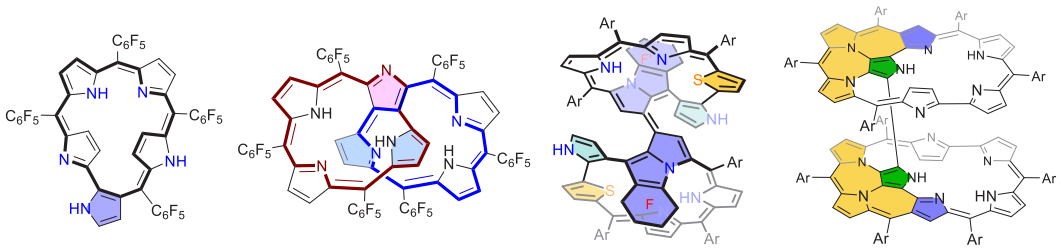


Fig. 1. Molecular structures of porphyrinoid monomers and dimers with tunable aromaticity.

REFERENCES

[1] Tanaka, T.; Osuka, A. *Chem. Rev.* **2017**, *117*, 2584-2640.

[2] (a) Nakai, A.; Tanaka, T.; Osuka, A., *Angew. Chem. Int. Ed.* **2023,** *62*, e202302662; (b) Luo, F.; Liu, L.; Wu, H.; Xu, L.; Rao, Y.; Zhou, M.; Osuka, A.; Song, J., *Nat. Commun.* **2023,** *14*, 5028; (c) Nakai, A.; Kim, J.; Tanaka, T.; Kim, D.; Osuka, A., *Angew. Chem. Int. Ed.* **2021,** *60*, 26540–26544 ; (d) Kino, S.; Ukai, S.; Fukui, N.; Haruki, R.; Kumai, R.; Wang, Q.; Horike, S.; Phung, Q. M.; Sundholm, D.; Shinokubo, H. *J. Am. Chem. Soc.* **2024**, *146*, 9311- 9317; (e) Sarma, T.; Kim, G.; Sen, S.; Cha, W. Y.; Duan, Z.; Moore, M. D.; Lynch, V. M.; Zhang, Z.; Kim, D.; Sessler, J. L. *J. Am. Chem. Soc.* **2018**, *140*, 12111-12119; (f) Hong, Y. S.; Oh, J.; Sung, Y. M.; Tanaka, Y.; Osuka, A.; Kim, D. *Angew. Chem. Int. Ed.* **2017**, *56*, 2932-2936.

[3] (a) Li, Q.; Ishida, M.; Kai, H.; Gu, T.; Li, C.; Li, X.; Baryshnikov, G.; Liang, X.; Zhu, W.; Ågren, H.; Furuta, H.; Xie, Y. *Angew. Chem. Int. Ed.* **2019**, *58*, 5925-5929 ; (b) Li, Q.; Ishida, M.; Wang, Y.; Li, C.; Baryshnikov, G.; Zhu, B.; Sha, F.; Wu, X.; Ågren, H.; Furuta, H.; Xie, Y. *Angew. Chem. Int. Ed.* **2023**, *62*, e202212174.

[4] Toganoh, M.; Furuta, H. *Chem. Rev.* **2022**, *122*, 8313-8437.

[5] (a) Li, Q.; Li, C.; Kim, J.; Ishida, M.; Li, X.; Gu, T.; Liang, X.; Zhu, W.; Ågren, H.; Kim, D.; Furuta, H.; Xie, Y. *J. Am. Chem. Soc.* **2019**, *141*, 5294-5302 ; (b) Li, Q.; Li, C.; Baryshnikov, G.; Ding, Y.; Zhao, C.; Gu, T.; Sha, F.; Liang, X.; Zhu, W.; Wu, X.; Ågren, H.; Sessler, J. L.; Xie, Y. *Nat. Commun.* **2020**, *11*, 5289; (c) Li, Q.; Ishida, M.; Li, C.; Baryshnikov, G.; Sha, F.; Zhu, B.; Wu, X.; Ågren, H.; Furuta, H.; Xie, Y. *CCS Chem.* **2023**, *5*, 1332-1342; (d) Huang, Y.; Zhu, B.; Li, S.; Baryshnikov, G.; Wang, H.; Li, C.; Ågren, H.; Jiang, J.; Xie, Y.; Li, Q. *J. Am. Chem. Soc.* **2025**, *147*, 28161-28172 ; (e) Xie, Y.; Su, G.; Ishida, M.; Zhu, B.; Baryshnikov, G.; Sha, F.; Li, C.; Wu, X.; Ågren, H.; Furuta, H.; Li, Q. *J. Am. Chem. Soc.* **2025**, *147*, 5368-5376.

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Development of Supramolecular and Bioorthogonal Approaches to Overcome the Challenges of Photodynamic Therapy

Evelyn Y. Xue and Dennis K. P. Ng*

Department of Chemistry, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China

Photodynamic therapy (PDT) is a clinically approved treatment modality for a range of localized and superficial cancers. It utilizes light to excite a photosensitizer localized within malignant tumors, generating cytotoxic reactive oxygen species (ROS) through interactions with endogenous oxygen. As the three components are individually nontoxic, the treatment is minimally invasive and has less systemic toxicity than traditional anticancer therapies. However, PDT still faces several limitations that hinder its clinical use. In particular, the low tumor selectivity and poor pharmacokinetics of most of the currently used photosensitizing drugs are problematic, leading to prolonged photosensitivity after the PDT treatment. We will discuss our recent research advancements in overcoming these challenges through the application of supramolecular and bioorthogonal chemistry.[1-3] By utilizing supramolecular and bioorthogonal approaches, we aim to achieve tumor-targeted photodynamic therapy. Furthermore, we have made significant progress in suppressing the photosensitivity of residual photosensitizers post-PDT treatment using bioorthogonal techniques.[4] These innovative strategies have the potential to enhance the selectivity and safety of PDT for cancer treatment.

REFERENCES

1. Xue, E. Y.; Shi, W. J.; Fong, W. P.; Ng, D. K. P.* Targeted delivery and site-specific activation of β-cyclodextrin-conjugated photosensitizers for photodynamic therapy through a supramolecular bio-orthogonal approach. *Journal of Medicinal Chemistry*, **202**1, *64*, 15461-15476.
2. Xue, E. Y.; Yang, C.; Fong, W. P.; Ng, D. K. P.* Site-specific displacement-driven activation of supramolecular photosensitizing nanoassemblies for antitumoral photodynamic therapy. *ACS Applied Materials & Interfaces*, **2022**, *14*, 14903-14915.
3. Xiong, J.[#]; Xue, E. Y.[#]; Wu, Q.; Lo, P. C.; Ng, D. K. P.* A tetrazine-responsive isonitrile-caged photosensitiser for site-specific photodynamic therapy. *Journal of Controlled Release*, **2023**, *353*, 663-674.
4. Xue, E. Y.; Yang, C.; Zhou, Y.; Ng, D. K. P.* A Bioorthogonal Antidote Against the Photosensitivity after Photodynamic Therapy. *Advanced Science*, **2024**, *11*, 2306207.

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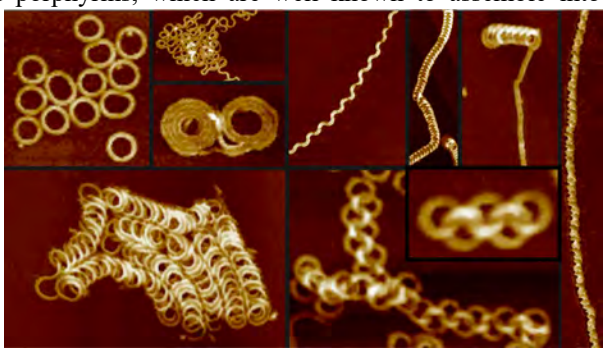
Curvature-Emergent Supramolecular Polymerization of Chlorophylls and Porphyrins

Shiki Yagai[a]

[a]*Institute for Advanced Academic Research(IAAR), Chiba University, Department of Applied Chemistry and Biotechnology, Graduate School of Engineering, Chiba University*

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Insights gained from the evolution of structural sophistication in covalent polymer chemistry provide a valuable framework for considering future directions in supramolecular polymer science.[1] Extensive studies over many decades have shown that deliberate control over polymer topology—ranging from helical and cyclic motifs to more complex hierarchical architectures—can dramatically broaden material functions. This prompts a fundamental question: can assemblies (supramolecular polymers) formed through reversible, non-covalent interactions be guided with a comparable level of structural precision? Furthermore, what types of emergent properties become accessible when such hierarchical organization is intentionally designed rather than incidentally formed? In this presentation, based on the concept of *curvature-emergent supramolecular polymerization*, we will explore how molecular design strategies can preprogram curvature into supramolecular motifs, thereby promoting hierarchical assembly and opening pathways to previously inaccessible functionalities. To date, we have successfully realized two distinct curvature-evergent self-assembly systems: a barbituric acid-based system[2-6] and a scissor-shaped molecular system.[7-9] A particularly important challenge for us is to extend the concept of curvature-emergent supramolecular polymerization based on the established molecular design to photofunctional chromophores such as chlorophylls and porphyrins, which are well known to assemble into curved architectures in nature. These chromophores generally exhibit strong aggregation tendencies, making controlled self-assembly difficult. Nevertheless, recent studies have begun to reveal several promising design principles and assembly strategies that may allow their aggregation behavior to be guided in a more controlled manner.[10-12] In this presentation, we will also introduce emerging insights along these lines.



REFERENCES

1. T. Aida, E.W. Meijer, *Isr. J. Chem.* **2020**, 60, 33.
2. S. Datta, Y. Kato, et al., *Nature*, **2020**, 583, 400.
3. S. Yagai, Y. Kitamoto, S. Datta, B. Adhikari, *Acc. Chem. Res.* **2019**, 52, 1325
4. S. Datta, S. Takahashi, S. Yagai, *Acc. Mater. Res.* **2022**, 3, 259
5. S. Datta, H. Itabashi, T. Saito, S. Yagai, *Nat. Chem.* **2025**, 17, 477
6. K. Tamaki, *Chem* **2026**, *12*, 102818.
7. T. Saito, et al., *J. Am. Chem. Soc.* **2023**, *145*, 443
8. T. Saito, et al., *Nat. Nanotechnol.* **2025**, 20, 825
9. T. Aizawa, et al., *submitted.*
10. R. Kudo, *et al., Chem. Commun.* **2025**, *61*, 8427.
11. R. Kudo, *et al., Org. Chem. Front.* **2024**, *11*, 6304-6310.
12. R. Kawai, *et al., under revision.*

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Solvent-Desorption-Induced Single-Crystal-to-Single-Crystal Transformation of Tetrabenzoporphyrin Leading to "Layered Herringbone Superlattice"

Miyazaki Kazuya [a], Keitaro Yamamoto[a], Hiroko Yamada[a]

[a]*Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*

In organic electronics, molecular packing is the primary determinant of charge transport performance. While polymorphism is a ubiquitous phenomenon, experimentally accessible structures are typically restricted to thermodynamically stable phases formed under equilibrium conditions.
In this study, we report a remarkable single-crystal-to-single-crystal (SCSC) transformation of 5,15-bisphenyl-tetrabenzoporphyrin (**Ph-BP**) triggered by the removal of intercalated *o*-dichlorobenzene (*o*-DCB) molecules [1]. X-ray crystallographic analysis reveals that this transformation induces a 90° rotation of the π-stacking direction between adjacent molecular layers. This process yields a previously unobserved crystal phase characterized by a periodic alternation of two distinct herringbone packing motifs, which we term a "layered herringbone superlattice." To evaluate the electronic impact of this transformation, we fabricated single-crystal organic field-effect transistors (OFETs) on Si/SiO_2 substrates. The superlattice phase exhibited an exceptional hole mobility of up to 11.3 $cm^2\ V^{-1}\ s^{-1}$, significantly outperforming the conventional thermodynamically stable polymorph of **Ph-BP**. This approach opens a new collective pathway to designing high-performance porphyrin-based semiconductors by navigating the complex landscape of metastable crystalline states.

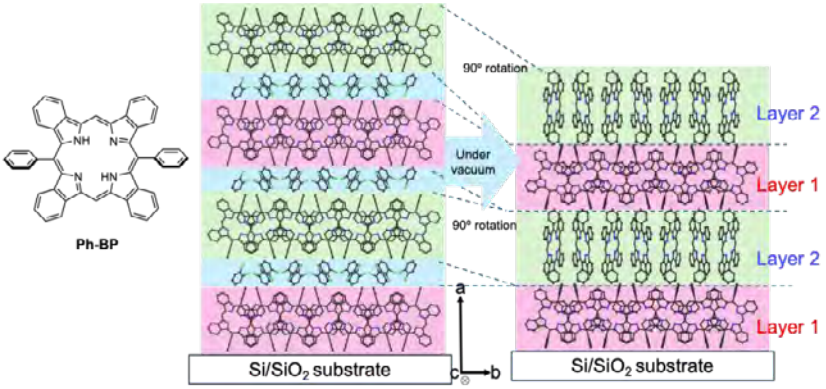


Figure. SCSC phase transformation of **Ph-BP** to "layered herringbone superlattice".

REFERENCES

1. K. Miyazaki, K. Yamamoto,* M. Yamauchi, Y. Mizuhata, H. Matsuda, N. Shioya, T. Hasegawa, H. Yamada*, Solvent-Desorption-Driven Superlattice Formation Yielding a High-Performance Porphyrin-Based Organic Semiconductor, *submitted*.

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Structure-Reactivity Relationship Studies of Monocationic μ-Nitrido-Bridged Iron Porphyrinoid Dimers

Yasuyuki Yamada[a] **and Kentaro Tanaka**[b]

[a] *Department of Biotechnology and Chemistry, Faculty of Engineering, Kindai University (Japan)*
[b] *Department of Chemistry, Graduate School of Science, Nagoya University (Japan)*

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μ-Nitrido-bridged dimers of metallo-porphyrinoids are a unique class of metallo-porphyrinoids. μ-Nitrido-bridged iron phthalocyanine dimers have attracted the interest of chemists due to their unique structures, the high oxidation states of their iron ions, and their applications in the catalytic conversion of small gaseous molecules, such as CH_4.[Ref. 1] The electronic structure of the phthalocyanine ring(s) was demonstrated to be an important factor in determining the reactivity of their catalytic oxidation reactions. [Ref. 1, 2] Therefore, replacing the phthalocyanine ring(s) with the other kinds of porphyrinoid(s) should dramatically change the electronic structures and oxidation activities.

In this study, we synthesized and characterized several different monocationic μ-nitrido-bridged iron porphyrinoid dimers (see **Fig. 1**) by using ^{1}H-NMR, UV-Vis spectroscopy, X-ray structural analysis, and electrochemical measurements. [Ref. 3] Detail on the CH_4 oxidation activities will also be presented.

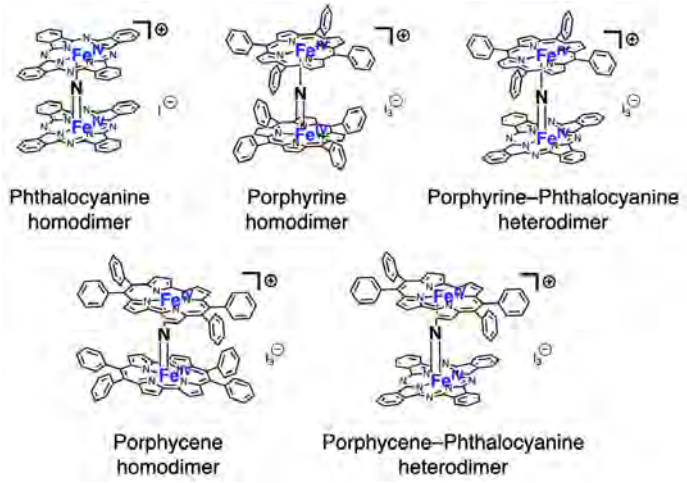


Fig. 1 Monocationic μ-nitrido-bridged iron porphyrinoid dimers synthesized in this study.

REFERENCES

1. P. Afanasiev and A. B. Sorokin, *Acc. Chem. Res. 49*, 583–593, **2016**.
2. (a) A. B. Sorokin, *et al. Chem. Sci., 6*, 5063–5075, **2015**, (b) Y. Yamada and K. Tanaka *et al.*: *New. J. Chem., 44*, 19179–19183, **2020**. *Dalton Trans.*, *50*, 6718–6724, **2021**. *JACS Au*, *3*, 823–833, **2023**.
3. Y. Yamada and K. Tanaka *et al.* : *Dalton Trans.*, *50*, 16775–16781, **2021**. *Catal. Sci. & Technol., 13*, 1725–1734, **2023**. *Catal. Sci. & Technol., 14*, 4854–4859, **2024**.

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An Exploratory Approach to Mitochondria-Targeted Photomedicine Using Porphyrinoid-Encapsulated Lipid Nanoparticles

Yuma Yamada [a]

[a] *Faculty of Pharmaceutical Sciences, Hokkaido University, Sapporo, Japan*

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Mitochondria play central roles in cellular energy metabolism, redox regulation, and apoptosis, and mitochondrial dysfunction is closely associated with a wide range of diseases, including cancer, cardiovascular disorders, and mitochondrial genetic diseases. These characteristics make mitochondria an attractive intracellular target for therapeutic intervention. However, effective and selective drug delivery to mitochondria remains a major challenge, as most previously reported mitochondrial drug delivery system (DDS) strategies have faced multiple limitations, including inefficient cellular internalization, strict size and physicochemical constraints on cargos, the requirement for chemical modification of functional molecules, and the loss of cargo activity during delivery.

To overcome these challenges, we developed an innovative mitochondria-targeted lipid nanoparticle (LNP) system, termed the MITO-Porter, which employs a membrane fusion–based delivery mechanism [1]. The MITO-Porter is composed of mitochondria-fusogenic lipids and the cell-penetrating peptide octaarginine (R8), enabling stepwise intracellular trafficking that includes cellular uptake *via* macropinocytosis, endosomal escape, mitochondrial binding through electrostatic interactions, and direct cargo delivery into mitochondria *via* membrane fusion. This strategy allows the mitochondrial delivery of diverse functional cargos independent of their size and physicochemical properties, while preserving their biological activity without chemical modification. Using this approach, we have demonstrated efficient mitochondrial delivery of anticancer drugs and achieved significant antitumor effects in drug-resistant cancer cells as well as in tumor-bearing animal models, highlighting the potential of this platform for overcoming therapeutic resistance associated with conventional nuclear- or cytosol-targeted anticancer therapies [2].

In addition to chemotherapy, we have applied the MITO-Porter system to mitochondria-targeted photodynamic therapy (PDT), in which the precise subcellular localization of photosensitizers is critical for maximizing therapeutic efficacy. By delivering porphyrin-based photosensitizers directly to mitochondria using LNPs, we achieved highly efficient photoinduced mitochondrial damage, including depolarization of the mitochondrial membrane potential and subsequent induction of apoptosis. Notably, this strategy enabled cancer cell death at markedly lower photosensitizer doses and light irradiation levels compared with conventional PDT approaches. These effects were validated both in vitro and in vivo using tumor-bearing mouse models, demonstrating robust therapeutic efficacy with minimal off-target toxicity and damage to surrounding tissues [3, 4]. Overall, the MITO-Porter LNP system represents a versatile and expandable platform for mitochondria-targeted drug delivery and phototherapy. This organelle-specific intervention strategy provides new opportunities for the development of innovative, academia-originated therapeutic approaches aimed at overcoming drug resistance and improving the precision and safety of next-generation nanomedicine.

REFERENCES

1. Yamada Y. et al., *Biochim. Biophys. Acta*, 1778, 423-432 (2008)
2. Yamada Y. et al., *Adv. Drug Deliv. Rev.*, 154-155, 187-209 (2020).
3. Satrialdi et al., *Chem. Commun*., 56, 1145–1148 (2020)
4. Satrialdi et al., *Nanoscale Adv.*, 3, 5919–5927 (2021).

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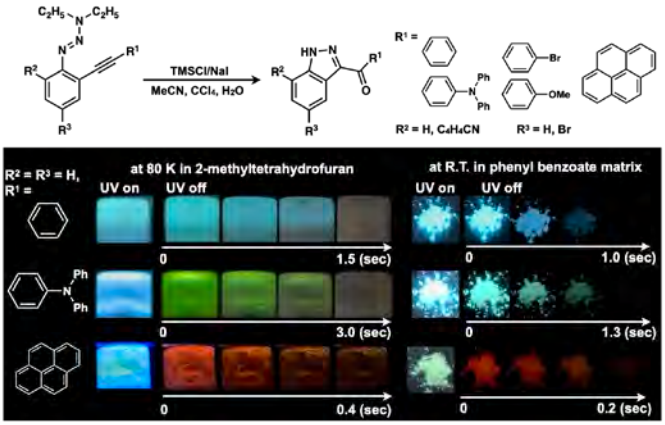


Mild Construction of Carbonylated Indazole Frameworks for Functional Molecular Design

Ryohei Yamakado

[a] *Graduate School of Organic Materials Science, Yamagata University*

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Nitrogen-containing aromatic compounds play central roles in pharmaceuticals, functional materials, and optoelectronic systems, where subtle variations in heteroaromatic frameworks critically govern electronic structure and excited-state dynamics. Among them, indazole derivatives represent an underexplored class of *N*-heteroaromatics compared with other heterocycles such as pyrrole, imidazole, and benzimidazole, despite their unique tautomerism, hydrogen-bonding ability, and potential for photofunctional applications. However, limited synthetic accessibility has long hindered systematic investigations of indazole-based functional molecules.

Herein, I will present our recent progress on the mild and versatile synthesis of carbonylated indazole derivatives and their application to photofunctional molecular design. We developed an azonium-mediated cyclisation of triazene precursors that enables efficient access to 3-(arylcarbonyl)-1*H*-indazole frameworks under mild, transition-metal-free conditions.[1] This strategy allows flexible introduction of diverse ketoaryl units while preserving the indazole core, providing a general platform for precise structural and electronic modulation.

The resulting indazole derivatives exhibit rich excited-state behavior. By tuning the ketoaryl substituents, the phosphorescence color can be widely modulated, and dual-emission and multi-component phosphorescence are realized at low temperatures. The emission characteristics are rationalized by theoretical analyses, which reveal how the interplay between (n,π*) and (π,π*) excited states, as well as substituent-dependent singlet–triplet energy gaps, governs intersystem crossing pathways. Furthermore, dispersion of the indazole derivatives in an appropriate host matrix enables room-temperature phosphorescence with distinct color variations, highlighting the strong coupling between the indazole framework and its molecular environment.[2]

Beyond isolated molecules, I will also introduce our ongoing efforts toward indazole-based supramolecular assemblies and polymeric systems, demonstrating how the indazole scaffold can serve as a modular building block for hierarchical organization and emergent photophysical functions in condensed states.

REFERENCES

1. Kuroyanagi, S.; Kikuchi, S.; Sumikoshi, S.; Uwano, M.; Chiba, T.; Yamakado, R.*; Okada, S. *Asian J. Org. Chem.* **2022**, *11*(11), e202200423.
2. Moriyama, T.; Kobayashi, R.; Chiba, T.; Okada, S.; Yamakado, R.* *Org. Biomol. Chem.* **2025**, *23*(20), 4902–4908.

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Plasticity of Pigment Composition and Spectroscopic Properties in Photosystem I of *Acaryochloris marina* Induced by Oxygen-Dependent Regulation of Chlorophyll *d* Biosynthesis

Kai Funahashi[a], Yuki Tsuzuki[a], Sorachi Katayama[a], Ibuki Y. Takahashi[b], Ryo Nagao[b],Yuichi Fujita[a], and Haruki Yamamoto[a]

[a]*Graduate School of Bioagricultural Sciences, Nagoya University, Nagoya, Japan*
[b]*Graduate School of Integrated Science and Technology, Shizuoka University, Shizuoka, Japan*

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Acaryochloris marina is a unique cyanobacterium that primarily utilizes chlorophyll (Chl) *d* as its major photosynthetic pigment, enabling the capture of far-red light up to ~710 nm. The strategy is considered an evolutionary strategy to utilize longer-wavelength solar energy that remains unused by Chl-*a*-carrying photosynthetic organisms. Despite its significance, the biosynthetic pathway of Chl *d* and the mechanisms governing its incorporation into photosynthetic complexes, particularly photosystem I (PSI), remain largely elusive. Previous studies have suggested that formylation at the C3 position, a key step in Chl *d* synthesis, is catalyzed by an oxygen-dependent oxygenase [1]. We previously demonstrated that Chl *d* biosynthesis can occur in a light-independent manner. Furthermore, we discovered that Chl *a*, a precursor of Chl *d*, accumulates significantly under dark-heterotrophic conditions [2].

In this study, we investigated the plasticity of pigment binding within the PSI complex by manipulating oxygen availability to suppress Chl *d* accumulation. Chl *a* accumulation was compared between two dark-heterotrophic conditions: shaking culture and static culture. We found that significant Chl *a* accumulation and a concomitant decrease in Chl *d* occurred only in the static culture, where oxygen supply is more severely limited. Interestingly, when the static culture (oxygen-limited cells) with Chl *a* accumulation was shifted back to shaking (oxygen-sufficient) conditions, the Chl *a* level rapidly decreased. This reversible physiological response provides further evidence supporting the hypothesis that C3-formylation in Chl *d* biosynthesis is oxygen-dependent.

We purified PSI complexes from *A. marina* cells grown under oxygen-limited conditions and characterized their biochemical and spectroscopic properties. HPLC analysis revealed that the Chl *a/d* ratio in the purified PSI was significantly higher than that in control cells grown under oxygen-sufficient conditions. Spectroscopic analysis of the PSI complexes showed a blue shift in the Q_y absorption band and altered low-temperature fluorescence emission. Recent structural studies have highlighted the diversity of PSI architectures among *Acaryochloris* species, including variations in oligomeric states and the presence of low-energy Chl *d* clusters ("red Chls") [3, 4]. Our results suggest that, under conditions of limited Chl *d* supply caused by low oxygen, the accumulated precursor Chl *a* can functionally substitute for Chl *d* at specific binding sites within the PSI complex. These findings demonstrate a remarkable degree of plasticity in the pigment-protein interactions of PSI and provide significant insights into how environmental oxygen levels and pigment availability influence the assembly and efficiency of far-red light-harvesting systems.

REFERENCES

1. Schliep, M., et al., *J. Biol. Chem.,* 285, 28450–28458 (2010).
2. Tsuzuki, Y., et al., *Plants,* 11, 915 (2022).
3. Nagao, R., et al., *Photosynth. Res.,* 157, 55–63 (2023).
4. Nagao, R., Yamamoto, H., et al., *Photosynth. Res.,* 161, 203–212 (2024).

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Isothianaphthene Quinoids with Controlled Diradical Character for NIR Phototransistors Using Porphyrin Hybrid Systems

Keitaro Yamamoto[a,b], Hiroko Yamada[a], Yutaka Ie[b]

[a] *Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*
[b] *The Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka 567-0047, Japan*

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Quinoidal π-conjugated systems have attracted significant attention as organic semiconductors owing to their narrow HOMO–LUMO energy gaps and unique electronic structures. These properties arise from the resonance between quinoidal and open-shell diradical forms. While this feature enhances π-electron delocalization, high diradical character often leads to molecular instability. In our previous studies, we demonstrated that the isothianaphthene scaffold effectively suppresses the diradical character of quinoidal oligothiophenes.
Based on this concept, we designed a series of extended quinoidal systems incorporating isothianaphthene units [1]. To synthesize the target molecules, we employed a precursor strategy utilizing retro-Diels–Alder reactions to generate isothianaphthene units. This approach allows the preparation of long quinoidal oligomers that are difficult to obtain through conventional synthetic routes. Experimental and theoretical studies indicated that the diradical character was well controlled and that the molecules exhibited high thermal stability. Photophysical measurements revealed that the extended quinoidal compounds exhibited red-shifted absorption in the near-infrared (NIR) region. Organic field-effect transistors (OFETs) based on these materials showed p-type or ambipolar charge transport behavior. Furthermore, bulk heterojunction devices composed of **5TQ-B5(EH)** as a donor and **2CF$_3$-BP** as an acceptor exhibited enhanced drain current under NIR light irradiation, demonstrating their potential as NIR-responsive organic phototransistors (OPTs).

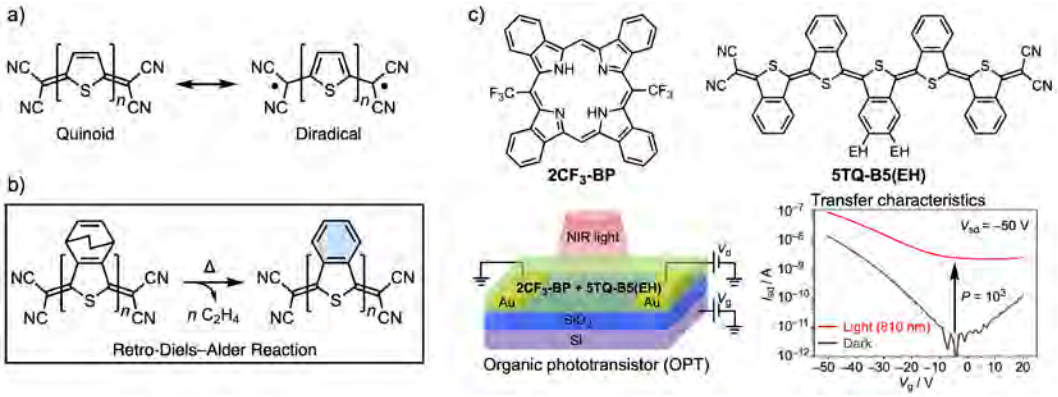


Figure 1. a) Resonance structure of quinoidal oligothiophenes. b) Synthesis of isothianaphthene quinoids via retro-Diels–Alder reaction. c) OPT application based on **2CF$_3$-BP** and **5TQ-B5(EH)**.

REFERENCES

1. Cross-conjugated isothianaphthene quinoids: a versatile strategy for controlling electronic structure, K. Yamamoto, S. M. Quintero, S. Jinnai, E. Jeong, K. Matsuo, M. Suzuki, H. Yamada, J. Casado*, Y. Ie*, *J. Mater. Chem. C* **2022**, *10*, 4424–4433.

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Redox Chemistry of β-Tetracyanoporphyrins: From Free-Base Isophlorins to Lanthanide Double-Decker Complexes

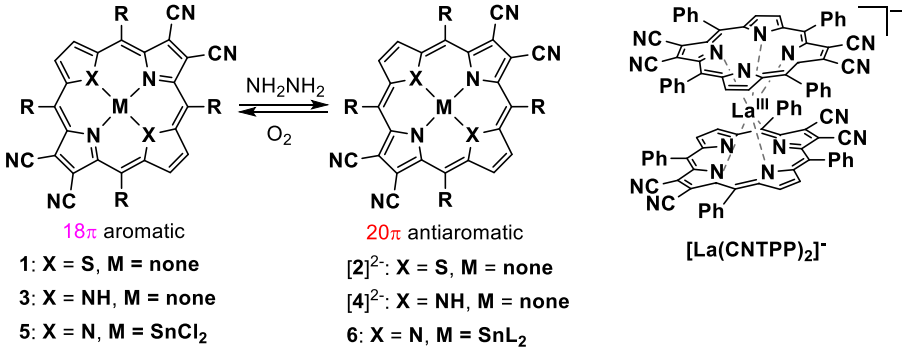
Ken-ichi Yamashita[a,b], **Haruna Sugimura**[a], **Kana Nakajima**[a]

[a]*Department of Chemistry, Graduate School of Science, The University of Osaka*
[b]*Innovative Catalysis Science Division, Institute for Open and Transdisciplinary Research Initiatives (ICS-OTRI), The University of Osaka*

ORALS

Redox-induced aromatic-antiaromatic interconversion in cyclic π-systems offers unique opportunities to modulate molecular properties. We have systematically investigated β-tetracyanoporphyrins (CNTPPs) with high reduction potentials, enabling stabilization of two-electron reduced antiaromatic isophlorins and exploration of multiply-reduced states. This series spans different core-modification numbers (CMN = 0, 2) and metal coordination environments.

We synthesized β-tetracyano-21,23-dithiaporphyrin (**1**, CMN=2) and demonstrated reversible reduction to the antiaromatic isophlorin $[\mathbf{2}]^{2-}$. Cyclic voltammetry revealed two reversible reduction waves, and the transformation was achieved chemically using hydrazine under ambient conditions.[1] We then achieved free-base β-tetracyanoisophlorins ($[\mathbf{4}]^{2-}$, CMN=0)—the first without metallation or core modification.[2] X-ray crystallography, NMR spectroscopy, and theoretical calculations confirmed their antiaromaticity. Metal complexation further modulates the electrochemical properties. A Sn(IV) β-tetracyanoporphyrin complex **5** exhibited reduction potentials approximately 0.2 V more positive than the free-base ligand **3**, facilitating reduction to the corresponding isophlorin **6**.[3] The Sn(IV) isophlorin complex **6** showed enhanced antiaromaticity due to enforced planarity and remained air-stable, unlike previously reported Si(IV) and Ge(IV) analogues. Most recently, we synthesized a La^{III} double-decker complexe $[La(CNTPP)_2]^-$, which exhibits four reversible reduction waves at –1.02, –1.22, –1.59, and –1.85 V (vs. Fc/Fc^+)—approximately 1.3 V more positive than $[La(TPP)_2]^-$, enabling unprecedented four-electron reduction to the pentaanion. Spectroelectrochemistry revealed characteristic absorption changes during stepwise reduction. We will discuss how peripheral substitution, core modification, and metal coordination systematically control the electrochemical properties and redox behavior of these porphyrinoids.



REFERENCES

1. K. Yamashita, K. Nakajima, Y. Honda, T. Ogawa, *Chem. Eur. J.* **2020**, *26*, 3633–3640.
2. H. Sugimura, K. Nakajima, K. Yamashita, T. Ogawa, *Eur. J. Org. Chem.* **2022**, e202200747.
3. H. Sugimura, K. Nakajima, K. Yamashita, *Asian J. Org. Chem.* **2025**, *14*, e202400550.

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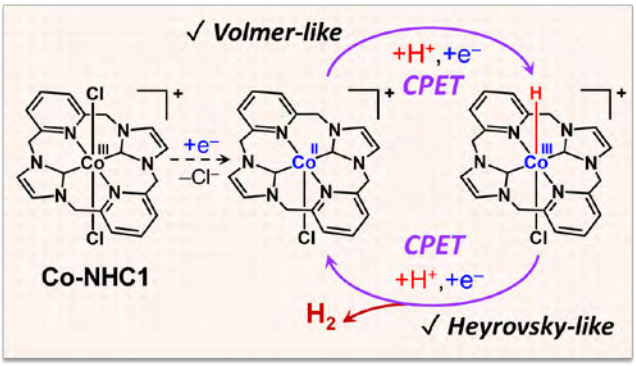
Photocatalytic Energy Conversion with Cobalt-NHC Catalysts

Kosei Yamauchi

Institute for Advanced Study, Kyushu University, Motooka 744, Nishi-ku, Fukuoka, Japan.

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Energy conversion based on H_2 evolution from water [1] and CO_2 reduction into various chemicals [2,3] are the key technologies to solve the global warming and shortage of fossil fuels. It is also important to couple these reduction reactions with water oxidation [4] to convert solar energy into chemical energy. In this context, we have studied on molecular photosystems in which hydrogen evolution reaction (HER) is driven by oxidative quenching of $[Ru^*(bpy)_3]^{2+}$. The photosystem comprises of EDTA, $[Ru(bpy)_3]^{2+}$, electron relay and the catalyst, where one-electron-reduced species of methylviologen MV^{2+} (i.e., $MV^{+}\bullet$) only has a driving force (DF) of 150 meV for HER at pH 5.0. Within these studies, we succeeded in demonstrating that a macrocyclic cobalt-NHC complex **Co-NHC1** (NHC: N-heterocyclic carbene) serves as a catalyst for HER using $MV^{+}\bullet$ as a reductant [1]. This is the first example of the 1st row transition metal complex showing the catalysis in this system. In addition, experimental and DFT results also reveal that a unique double CPET pathway is taken to evolve H_2 by **Co-NHC1** with substantially minimized reorganization energies [1]. This pathway can be viewed as related to the so-called Volmer-Heyrovsky mechanism adopted by some metals and is quite unique to **Co-NHC1**. Meanwhile, we have recently conducted the detailed analyses on the electrocatalysis of **Co-NHC1** for hydrogen evolution from water. Importantly, the catalytic rate by **Co-NHC1** has turned out to be extremely high even in neutral aqueous media [5]. Our recent finding includes the development of the highly efficient molecular system in photochemical H_2 evolution from alkaline water.



REFERENCES

1. K. Yamauchi*, K. Kawano, K. Yatsuzuka, K. Kawamura, M. Kan, K. Sakai*, *J. Am. Chem. Soc.,* **2025**, 147, 5602-5614 (***Supplementary Cover***).
2. D. Lee, K. Yamauchi*, K. Sakai*, *J. Am. Chem. Soc.*, **2024,** *146*, 31597-31611.
3. C. Liao, K. Yamauchi*, K. Sakai*, *ACS Catal.,* **2024**, *14*, 11131-11137.
4. Y. Aimoto, A. R. Parent*, K. Yamauchi*, K. Sakai*, *J. Am. Chem. Soc.*, **2024**, *146*, 16866-16877.
5. M. Kan, K. Yamauchi*, K. Sakai*, *ChemRxiv*, DOI: 10.26434/chemrxiv-2025-hwww9.

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Hydrogen-Bonded Tetrabenzoporphyrin Thin Films: Evaluation of Assembly Structure and Transistor Properties

Mitsuaki Yamauchi[a]

[a]*Institute for Chemical Research, KyotoUniversity*

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Organic semiconductor materials are regarded as an important class of functional materials due to their flexible and lightweight properties, and low-cost device fabrication processes, such as solution-processing methods. The improvement of charge-carrier mobility in organic thin-film transistors (OTFTs) is essential for achieving practical application levels. To enhance the mobility, researchers have explored optimal packing structures by modifying molecular structures and fine-tuning the van der Waals interactions, such as those between alkyl chains and π-conjugated cores. However, supramolecularly designed OTFTs incorporating hydrogen bonds have not been sufficiently developed, because of the reduced solubility caused by introducing hydrogen bond sites and the difficulty in controlling molecular orientations and packing structures.

Herein, we report a strategy for the formation of hydrogen-bonded supramolecular semiconductor thin films using the thermal precursor approach (Fig. 1a) [1,2]. As a model π-extended core unit, tetrabenzoporphyrin (**BP**) was selected because of its large, rigid π-surface that can form tight π-stacking, enabling efficient charge-carrier transport [3]. We designed a **BP** derivative bearing amide groups and dodecyl chains via phenyl linkages (**BPa**, Fig. 1b) and synthesized the corresponding precursor, bicyclo[2.2.2]octadiene-fused porphyrin derivative (**CPa**, Fig. 1b). As expected, a **CPa** film was prepared by drop-casting and thermally converted into the **BPa** film via the retro-Diels–Alder reaction, as confirmed by spectroscopic analyses. The hydrogen-bonded assembly structures of **CPa** and **BPa** in the film state were revealed by a combination of X-ray diffraction (XRD) and infrared p-polarized multiple-angle incidence resolution spectrometry (IR-pMAIRS) analyses. Moreover, we fabricated OTFTs exhibiting a high hole mobility of 0.25 $cm^2\ V^{-1}\ s^{-1}$ among hydrogen-bonded OTFTs reported to date. The high thermal stability of **BPa** films was confirmed, with device performance maintained in air up to 250 °C, attributed to the hydrogen-bonded networks.

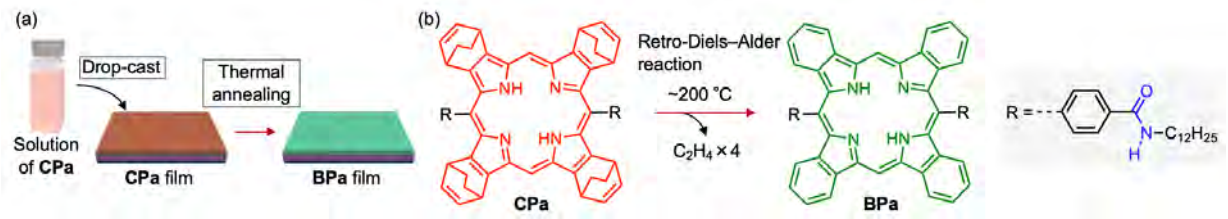


Fig. 1. (a) Fabrication method of thin films via thermal precursor approach. (b) Structures of **CPa** and **BPa**.

REFERENCES

1. K. Takahashi, B. Shan, X. Xu, S. Yang, T. Koganezawa, D. Kuzuhara, N. Aratani, M. Suzuki, Q. Miao, H. Yamada, *ACS Appl. Mater. Inter.* **2017**, *9*, 8211–8218.
2. S. Ueno, M. Yamauchi, N. Shioya, H. Matsuda, T. Hasegawa, K. Yamamoto, Y. Mizuhata, H. Yamada, *Angew. Chem. Int. Ed.* **2025**, *64*, e202425188.
3. S. Ueno, M. Yamauchi, H. Matsuda, N. Shioya, K. Yamamoto, Y. Mizuhata, T. Hasegawa, H. Yamada, *J. Mater. Chem. C* **2025**, *13*, 23766−23771.

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Temperature dependence of substrate inhibition in human Indoleamine 2,3-dioxygenase1

Sachiko Yanagisawa

Graduate School of Science, University of Hyogo, Koto 3-2-1, Kamigori-cho, Ako-gun, Hyogo 678-1297, Japan

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Human indoleamine 2,3-dioxygenase 1 (IDO) is a heme enzyme that catalyzes the incorporation of two oxygen atoms into L-tryptophan (L-Trp), resulting in its conversion to N-formylkynurenin (NFK). This enzyme plays a key role in the immune evasion process [1]. Therefore, inhibitors of this enzyme are expected to become promising cancer treatments, and research in this field is actively underway [2]. The reaction mechanism of IDO is also of interest. Spectroscopic experiments [3,4] and classic molecular dynamics and hybrid quantum mechanical and molecular mechanical (QM/MM) simulations [3] have indicated a two-step dioxygenation process involving a ferryl-oxo intermediate. Furthermore, IDO exhibits substrate inhibition, which is characterized by decreased activity at elevated substrate concentrations. Several mechanisms of substrate inhibition have been proposed [5,6]. Nevertheless, the mechanism of substrate inhibition remains to be fully elucidated. The present study focuses on IDO during substrate-inhibitory reactions and its thermodynamic behavior to improve understanding of substrate inhibition.

We measured the absorption spectra of IDO during the enzymatic reaction at two temperatures, under high substrate, L-Trp, concentrations, where substrate inhibition occurs. As a result, we found that the phase of substrate inhibition with slow NFK production was obtained more quickly at the higher temperature. However, the spectral species obtained during the reaction were the same at both temperatures. We also measured the enzymatic reaction rate at various L-Trp concentrations and temperatures with a constant oxygen concentration. Using Michaels-Menten fitting, we determined Michaelis constant (K_m) and inhibitor constant (K_i) values based on the L-Trp concentration-dependent reaction rate at various temperatures. As a result, K_m increased with temperature, whereas K_i decreased. Considering K_i as the dissociation constant of the substrate to a substrate inhibition site (S_i site), this result indicates that affinity of the substrate for the S_i site increases at higher temperatures. This implies that temperature-dependent conformational fluctuations around the S_i site are important for substrate binding. In addition, based on the temperature dependence of K_i, we obtained the thermodynamic parameters of the free energy change, the enthalpy change, and the entropy change associated with L-Trp binding to the S_i site. These values provide qualitative information about L-Trp binding to the S_i site. In the future, we will perform molecular dynamics simulations to fully understand substrate inhibition in IDO. Then, we will use our experimental data to evaluate the simulation results.

REFERENCES

1. G. C. Prendergast, *Nature* 478 (2011) 192–194.
2. U. F. Röhrig *et al*., *J. Med. Chem.* 64 (2021) 17690-17705
3. A. Lewis-Ballester *et al.*, *Proc. Natl. Acad. Sci. USA* 106 (2009) 17371-17376
4. S. Yanagisawa *et al.*, Chem. Lett., 39 (2010) 36-37
5. A. Lewis-Ballester *et al.*, *J. Am. Chem. Soc.* 140 (2018) 8518−8525.
6. A. O. Kolawole *et al.*, *Arch. Biochem. Biophys.* 570 (2015) 47– 57.

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Photo-Excited Porphyrins as a Platform for Spin Hyperpolarization: From Magnetic Resonance to Quantum Sensing

Nobuhiro Yanai[a]

[a]*Department of Chemistry, Graduate School of Science, The University of Tokyo, Japan*

Enhanced spin polarization can significantly increase the sensitivity of magnetic resonance techniques such as EPR, NMR, and MRI. Furthermore, in the context of quantum information science (QIS), the generation of spin polarization is important for initialization and for enhancing sensitivity in quantum computing and quantum sensing applications. When using electron spins in thermal equilibrium, high magnetic fields at very low temperatures are required to obtain large spin polarization. On the other hand, by using photoexcitation of chromophores, non-equilibrium large electron spin polarization can be obtained even at room temperature. Furthermore, quantum sensing based on optically detected magnetic resonance (ODMR) is possible with photoexcited chromophores.

To control the assembly structure of the excited state and to make it responsive to external stimuli, we used metal–organic frameworks (MOFs) as a platform. Porphyrin-based chromophores were densely arranged in the MOF structures as ligands. For example, we have also demonstrated the concept of light-harvesting spin polarization and effectively hyperpolarize radical electron spins by harvesting mobile excitons in MOFs.

Photochemically induced dynamic nuclear polarization (Photo-CIDNP) is a method to improve the sensitivity of NMR and MRI by light irradiation. Its major advantage over other DNP methods is that it does not require microwave irradiation. This feature would enable DNP in living cells and animals, in addition to DNP of biomolecules in action. This presentation reports progress on our new material developments for photo-CIDNP. To enable its use in biological systems, enhancing the sensitivity of ^{19}F via photo-CIDNP is beneficial. Screening over 200 combinations of candidate ^{19}F-labeled quenchers and dyes yielded an exceptionally high polarization exceeding 1%. Furthermore, we developed a photo-CIDNP chemical probe that turns on photo-CIDNP activity from an OFF state to an ON state by altering the quencher structure via an enzymatic reaction. This is expected to enable monitoring of specific diseases using photo-CIDNP-enhanced MRI signals.

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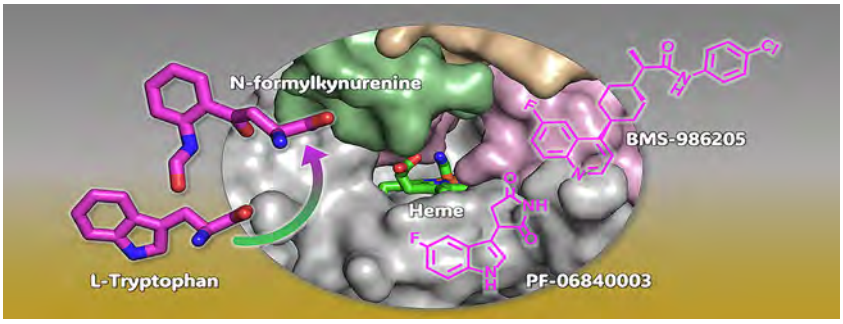
Molecular Determinants of Selective Inhibition of Human IDO1 and TDO

Syun-Ru Yeh

Department of Biochemistry, Albert Einstein College of Medicine, 1300 Morris Park Ave., Bronx, NY 10461

ORALS

Human tryptophan 2,3-dioxygenase (hTDO) and indoleamine 2,3-dioxygenase 1 (hIDO1) are heme-dependent enzymes that catalyze the first and rate-limiting step of the kynurenine pathway by converting L-tryptophan to N-formylkynurenine. Both enzymes have emerged as important targets in cancer immunotherapy; however, rational inhibitor design has been hindered by limited structural insight, particularly for hTDO. Here, we employ a set of hIDO1- and hTDO-selective inhibitors as structural probes, in combination with spectroscopic and crystallographic approaches, to investigate the molecular basis of inhibitor selectivity between the two enzymes. Our results reveal that, despite high structural similarity and sequence homology between the active sites of hIDO1 and hTDO, hIDO1 exhibits markedly greater conformational flexibility, enabling inhibitor binding through an induced-fit mechanism, whereas hTDO possesses a more rigid binding pocket that favors a lock-and-key mode of recognition. Together, these findings provide new insights to guide the structure-based design of selective and dual inhibitors targeting hIDO1 and/or hTDO.



REFERENCES

1. "Heme-based dioxygenases: Structure, function and dynamics." Geeraerts Z, Ishigami I, Gao Y, Yeh SR. J Inorg Biochem., 261, 112707, 2024. doi: 10.1016/j.jinorgbio.2024.112707.
2. "Structural Insights into Protein-Inhibitor Interactions in Human Tryptophan Dioxygenase."Geeraerts Z, Ishigami I, Lewis-Ballester A, Pham KN, Kozlova A, Mathieu C, Frédérick R, Yeh SR. J Med Chem. 67, 14543, 2024. doi: 10.1021/acs.jmedchem.4c01360.
3. "Conformational Plasticity in Human Heme-Based Dioxygenases." Pham KN, Lewis-Ballester A, Yeh SR. J Am Chem Soc. 143, 1836, 2021. doi: 10.1021/jacs.0c09970.
4. "Structural Basis of Inhibitor Selectivity in Human Indoleamine 2,3-Dioxygenase 1 and Tryptophan Dioxygenase" Pham KN, Lewis-Ballester A, Yeh SR. J Am Chem Soc. 141, 18771, 2019. doi: 10.1021/jacs.9b08871.
5. "Mapping the Binding Trajectory of a Suicide Inhibitor in Human Indoleamine 2,3-Dioxygenase 1." Pham KN, Yeh SR. J Am Chem Soc. 140, 14538, 2018. doi: 10.1021/jacs.8b07994.
6. "Inhibition Mechanisms of Human Indoleamine 2,3 Dioxygenase 1." Lewis-Ballester A, Karkashon S, Batabyal D, Poulos TL, Yeh SR. J Am Chem Soc. 140, 8518, 2018. doi: 10.1021/jacs.8b03691.
7. "Structural insights into substrate and inhibitor binding sites in human indoleamine 2,3-dioxygenase 1." Lewis-Ballester A, Pham KN, Batabyal D, Karkashon S, Bonanno JB, Poulos TL, Yeh SR. Nat Commun. 8, 1693, 2017. doi: 10.1038/s41467-017-01725-8.

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Recent Progress on Fluorescent Imaging Probes and Phototherapy

Juyoung Yoon[a,b]

[a]*Department of Chemistry and Nanoscience, Ewha Womans University, Seoul 03760, Korea*
[b]*Graduate Program in Innovative Biomaterials Convergence, Ewha Womans University, Seoul 03760, Korea*
E-mail: jyoon@ewha.ac.kr

Phototherapy, includes photodynamic therapy (PDT) and photothermal therapy (PTT), which combine light with an adequate wavelength and a chemical phototheranostic agent in the absence or presence of oxygen, possesses substantial potential for cancer treatment due to its significant specificity, extremely low invasiveness, flexible administration, and effective cancer therapy. Especially, smart photosensitizers (PSs) have recently attracted considerable attention due to their highly effective cancer therapeutic performance combined with improved biosafety [1]. Recent contributions from our group for this topic will be presented; enhanced synergistic photodynamic and photothermal therapy guided by photoacoustic imaging [2], a hypoxia-triggered bioreduction of hydrophilic type I photosensitizer for switchable in vivo photoacoustic imaging and cancer phototherapy [3], conversion of albumin into a BODIPY-like photosensitizer by a flick reaction, tumor accumulation and photodynamic therapy [4] and a photo-driven unimolecular immunostimulant for self-amplified pyroptosis and cGAS-STING pathway by destroying the pyroptosis checkpoint [5].

REFERENCES

1. Zhao Y-Y, Lu L, Jeong H, Kim H, Li X, Zhang H, Yoon J. *Chem. Soc. Rev.* 2025; **54**: 7749-7768.
2. Zhao Y-Y, Zhang X, Xu Y, Chen Z, Hwang B, Kim H, Liu H, Li X, Yoon J. *Angew. Chem. Int. Ed.* 2024; **63**: e202411514.
3. Zhao Y-Y, Xu Y, Zhang X, Chen Z, Kim H, Li X, Yoon J. *Angew. Chem. Int. Ed.* 2025; **64**: e202506412.
4. Yang M, Kim Y, Youn S-Y, Jeong H, Shirbhate M E, Uhm C, Kim G, Nam K T, Cha S-S, Kim K M, Yoon J. *Biomaterials* 2025; **313**: 122792.
5. Zeng S, Chen C, Guo Z, Qin C, Wang Y, Liu X, Li X, Jeong H, Hao Y, Zhou D, Long S, Wu Z, Wang J, Li H, Peng X, Yoon J. *Angew. Chem. Int. Ed.* 2025; **64**: e202513815.

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Application of Iron Phthalocyanine Dimers as Cathode-Active Materials for Rechargeable Batteries

Hirofumi Yoshikawa[a]

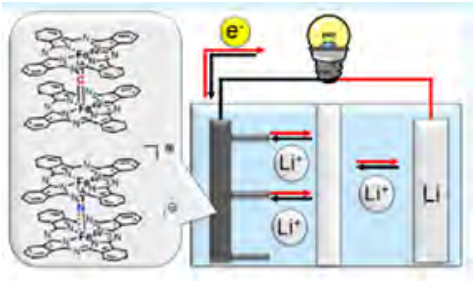
[a]*Kwansei Gakuin University*

ORALS

Phthalocyanines constitute an important class of artificial porphyrinoids that have attracted considerable attention because of their wide variety of applications in functionalmolecular devices and as luminescent dyes, medicinal dyes, and liquid crystals. In recent years, the application of phthalocya nines to electrode-active materials for rechargeable batteries has been of significant interest, mainly because some phthalocyanines show stable redox properties and enable multiple-electron storage despite a relatively small size.

μ -Heteroatom-bridged iron phthalocyanine dimers represent a unique class of metallophthalocyanines. It is known that carbon, nitrogen, or oxygen atoms can be stably incorporated between two iron phthalocyanines to form the corresponding μ -heteroatom-bridged iron phthalocyanine dimers. These dimers have attracted the interest of chemists because of their unique structures and the high oxidation states of their iron atoms, as well as their applications in the catalytic conversion of small gas molecules like CH_4. However, judging from their structures, they can store multiple electrons in their two cofacially stacked phthalocyanine rings and their two iron centers connected through a bridging atom. In these phthalocyanine dimers. Herein we measured these

Firstly, we compared the cyclic voltammograms of μ-nitrido-bridged and μ-carbido-bridged iron phthalocyanine dimers with no peripheral substituents [$(FePc)_2N^+ \cdot I^-$ and$(FePc)_2C$] in pyridine solution to confirm that both complexesshowed four quasi-reversible redox waves in the potential range between −2.2 and 0.1 V vs Fc/Fc+. We applied both complexesas the cathode-active material of rechargeable batteries. They showed discharge capacities of 60 mAh g−1 after 200 cycles, which is consistent with the theoretically calculated values. Thus, it was demonstrated that μ-heteroatom-bridged iron phthalocyanine dimers act as a good platform for active materials in rechargeable batteries. Their battery performances are not the best one at present, but the appropriate chemical modification of peripheral phthalo cyanine rings, such as the introduction of quinone units, would endow them with further multiredox capabilities. Especially, because redox-active μ-nitrido-bridged and μ-carbido-bridged dimers, which are more stable among phthalocyanine dimers, have been reported only for iron ions, incorporation of other central metal ions is effective to improve the battery performances. Moreover, both μ-carbido- and μ-nitrido bridged iron phthalocyanine dimers are expected to act as bipolar electroactive materials because of their stability against both reduction and oxidation.



REFERENCES

1. H. Yoshikawa et al., *ACS Appl. Mater. Interfaces* 2021, 13, 40612−40617

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Visible-Light-Driven Zn(II)porphyrin Catalysis in Natural Product Synthesis

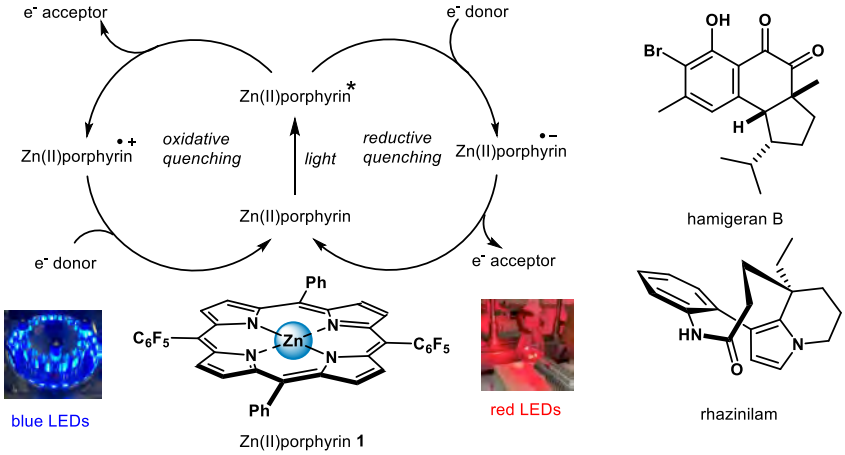
Takehiko Yoshimitsu

Division of Pharmaceutical Sciences, Graduate School of Medicine, Dentistry, and Pharmaceutical Sciences, Okayama University, 1-1-1 Tsushimanaka, Kita-ku, Okayama 700-8530, Japan.

ORALS

Porphyrins and metalloporphyrins have emerged as versatile visible-light photoredox catalysts that enable single-electron transfer (SET) and energy-transfer (ET) processes useful for organic synthesis. This presentation will describe our recent efforts toward the implementation of zinc(II)porphyrin **1**, a light-flexible catalyst compatible with both blue- and red-light excitation, in the total synthesis of natural products such as hamigeran B [1] and rhazinilam [2] (Scheme 1). In addition, its capability to promote a broad range of radical transformations, including a light-driven decarboxylative cascade reaction [3], a Giese reaction, and a homolytic aromatic substitution (HAS) reaction, will be discussed.

Scheme 1. Zn(II)porphyrin-catalyzed radical reactions driven by visible light



REFERENCES

1. Okanishi, Y.; Ishikawa, T.; Jinnouchi, T.; Hayashi, S.; Takanami, T.; Aoyama, H.; Yoshimitsu, T. *J. Org. Chem.* **2023**, *88*, 1085-1092.
2. Okanishi, Y.; Yotsumoto, Y.; Yoshimitsu, T. *Org. Lett*. **2025**, *27*, 5840-5845.
3. Okanishi, Y.; Takemoto, O.; Kawahara, S.;Hayashi, S.; Takanami, T.; Yoshimitsu, T. *Org. Lett.* **2024**, *26*, 3929-3934.

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Aromatic Micelles with Host Functions toward Aromatic Polymers

Michito Yoshizawa[a]

[a]*Laboratory for Chemistry and Life Science, Institute of Integrated Research, Institute of Science, Tokyo, Yokohama, Japan*

ORALS

Linear and spherical aromatic polymers are appealing materials. However, without attachment of multiple side chains, their applications have been largely limited to the solid state as mixtures due to complete insolubility. To unlock their utility and functions in solution, we report here the efficient solubilization of linear and spherical aromatic polymers without side chains, with ~lengths of 400 nm and ~100 nm, respectively, through encapsulation by aromatic micelles in water.[1,2] The micelles are composed of bent amphiphiles with two aromatic panels for efficient hydrophobic effect as well as π-π and CH-π interactions.[3,4] This method enables straightforward size fractionation of the spherical polymers via a centrifugation-filtration protocol, yielding highly monodisperse particles. Importantly, the resulting composites serve as aqueous, giant polycavity hosts that incorporate hydrocarbons and fluorescent dyes, thereby providing unique quaternary host-guest composites (Figure 1).[2]

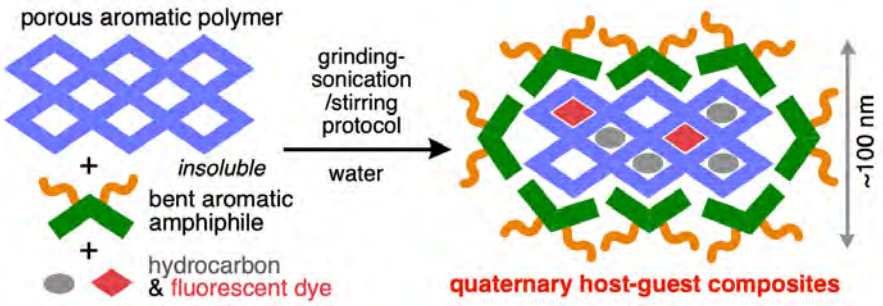


Figure 1. Preparation of quaternary host-guest composites via encapsulation of a spherical, porous aromatic polymer by an aromatic micelle in water.

REFERENCES

1. S. Aoyama, L. Catti, M. Yoshizawa, *Angew. Chem. Int. Ed.* **2023**, 62, e202306399.
2. S. Aoyama, L. Catti, M. Yoshizawa, *Chem* **2025**, 11, 102616.
3. (a) K. Kondo, A. Suzuki, M. Akita, M. Yoshizawa, *Angew. Chem. Int. Ed.* **2013**, 52, 2308–2312; (b) M. Yoshizawa, L. Catti, *Acc. Chem. Res.* 2019, 52, 2392–2404; (c) M. Yoshizawa, L. Catti, *Proc. Jpn. Acad., Ser.* B 2023, 99, 29–38.
4. (a) M. Endo, S. Aoyama, Y. Tsuchido, L. Catti, M. Yoshizawa, *Angew. Chem. Int. Ed.* **2024**, 63, e202404088; (b) Y. Hashimoto, Y. Tanaka, D. Suzuki, Y. Imai, M. Yoshizawa, *J. Am. Chem. Soc.* **2024**, 146, 23669–23673; (c) Y. Hashimoto, Y. Tanaka, S.-Y. Liu, H. Shinokubo, M. Yoshizawa, *J. Am. Chem. Soc.* **2025**, 147, 23060–23067; (d) D. Kidoh, L. Catti, S. Aoyama, D. Tauchi, M. Hasegawa, M. Yoshizawa, *Angew. Chem. Int. Ed.* **2025**, 64, in press.

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Greener Phthalocyanines: From Sustainable Synthetic Design to Functional Interfaces and Devices

Gloria Zanotti[a]

[a] *Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), Strada provinciale 35d/9, 00010 Montelibretti, Rm (Italy)*

ORALS

Phthalocyanines remain a cornerstone class of functional molecular materials, owing to their structural versatility, rich electronic properties, and broad applicability in energy, environmental, and sensing technologies. Although industrial processes are generally optimized for large-scale production, many laboratory-scale synthetic routes still rely on solvent-intensive, multistep protocols, motivating the development of more sustainable synthetic strategies.[1] This contribution discusses how sustainable synthetic design can be leveraged not only to reduce the environmental and economic footprint of phthalocyanine chemistry but also to broaden the functional and processing opportunities of phthalocyanine-based materials.[2]

Starting from the implementation of green chemistry principles, including strategies to reduce the Environmental factor (E-factor),[3] a widely adopted metric for assessing waste generation in chemical synthesis, practical and potentially scalable synthetic routes to unsubstituted and substituted phthalocyanines are presented that rely on two main design elements: (i) the use of alternative, more sustainable reaction media, such as low-molecular-weight polyols and PEG-based liquid-phase systems, and (ii) pot-economical sequences. Recent and ongoing work underpinning this contribution demonstrates that these elements can be integrated into unified synthetic platforms that address solvent sustainability and multistep compatibility simultaneously. In this context, PEG-400 is discussed as a representative case study enabling the combination of metal-templated phthalonitrile cyclotetramerization with subsequent catalytic functionalization steps performed directly in the same reaction environment. Such integrated one-pot and telescopic strategies allow multiple, chemically distinct transformations to be orchestrated without intermediate isolation. These methodologies are critically assessed for efficiency, scope, and reproducibility, with particular attention to the extent to which synthetic simplification can coexist with fine structural control. Beyond synthesis, this contribution emphasizes how these greener approaches increase the relevance of phthalocyanines for functional interfaces and device architectures by addressing sustainability- and cost-related constraints associated with their practical use. Selected representative examples illustrate their implementation as active layers or interfacial materials in energy-related devices, such as photovoltaics,[4] as well as in environmental applications, including CO_2 conversion,[5] and sensing of aquatic pollutants. By bridging sustainable molecular design with interface engineering and device-relevant properties, this contribution outlines a coherent framework in which greener phthalocyanine chemistry facilitates the development and integration of phthalocyanine-based materials in functional systems for energy and environmental technologies.

REFERENCES

1. G. Zanotti et al. *Chem. Eur. J.* **2024**; 30: e202400908; DOI: 10.1002/chem.202400908.
2. F. Palmeri et al. *Org. Chem. Front.* **2026**; DOI: 10.1039/D5QO01267H.
3. R.A. Sheldon et al. *Green Chem.* **2023**; 25: 1704-1728; DOI: 10.1039/D2GC04747K.
4 S.K. Podapangi, L. Mancini, D. Takhellambam et al. *ChemRxiv*, **2025**; DOI: 10.26434/chemrxiv-2025-8ctgt. (preprint)
5 G. Zanotti et al. *Chem. Eur. J* **2025**; 0:e02264; DOI: 10.1002/chem.202502264.

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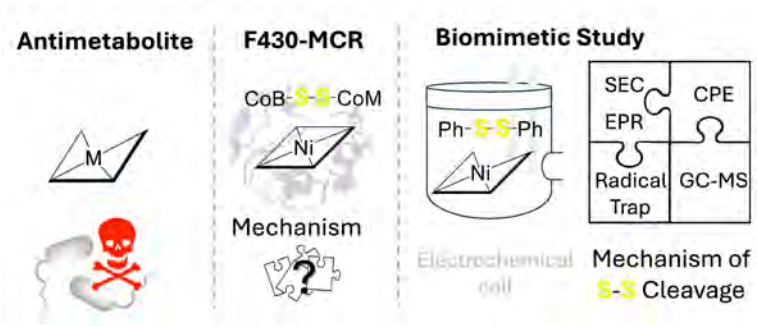
Metal Substitution and Bioactivity in Vitamin B_{12} Derivatives: From Biomimetic Catalysis to Antimicrobial Function

Kaifeng Wang, Samira Amini, Christopher Brening, Daniela Mestizo, Felix Zelder

Department of Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland.

ORALS

My group`s research examines the structure and function of tetrapyrrole cofactors, focusing on vitamin B_{12} and the nickel-containing cofactor F_{430} that mediate key microbial redox processes. We synthesized B_{12} derivatives incorporating nickel and copper to probe how metal substitution affects electronic structure and catalytic behavior [1]. Nickel–B_{12} derivatives served as biomimetic models of F_{430}, with electrochemical studies revealing parallels to radical-mediated anaerobic methane oxidation [2].



Building on these insights, modified B_{12} derivatives were evaluated as antimicrobial agents against *Lactobacillus delbrueckii*, *Listeria monocytogenes*, and other microorganisms. Several compounds displayed notable inhibitory activity toward *L. delbrueckii*, demonstrating that targeted corrin modification can yield B_{12}-based scaffolds with antibiotic potential. This work connects metallocofactor design to new strategies in antimicrobial development [3].

Financial support by the University of Zurich and the Schweizerischer Nationalfonds (SNFS-200021_197358) is acknowledged. We acknowledge also generous gifts of B_{12} from Prof. em. Bernhard Kräutler (University of Innsbruck) as well as from Prof. em. Bernhard Jaun (ETH Zurich).

REFERENCES

1. C. Brenig, L. Prieto, R. Oetterli and F. Zelder, *Angew. Chem. Int. Ed.*, 2018, **57**, 16308-16312.

2. S. Amini, K. Oppelt, O. Blacque, M. Agrachev, G. Jeschke and F. Zelder, *Chem. Sci.*, 2025, DOI: 10.1039/D4SC08416K, 4290-4294.

3. C. Brenig, P. D. Mestizo and F. Zelder, *RSC Adv.*, 2022, **12**, 28553-28559.

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Molecular structure and thermodynamic properties of tetrapyrrole macrocycle complexes

Yuriy A. Zhabanov

Ivanovo State University of Chemistry and Technology, Research Institute of Chemistry of Macroheterocyclic Compounds, 153000 Ivanovo, Russia

ORALS

The expansion of practical application areas for tetrapyrrole macrocycles, such as nonlinear optics, production of semiconductor and liquid crystal materials, and sensor devices, requires not only broadening the spectrum of their molecular architecture and methods of its construction but also expanding research into the relationship between the geometric and electronic structure of molecules and their reactivity and spectroscopic properties. This serves as the fundamental basis for implementing the processes of developing and obtaining new materials with desired properties.

This work presents an experimental and theoretical investigation of the geometric and electronic structure of macrocycle molecules with the aim of establishing and theoretically explaining general patterns in their structure. A set of theoretical and experimental methods was used for a comprehensive study of the structure and energetics of macroheterocyclic compounds. The vapor pressure and thermodynamic characteristics of macrocycles were determined by high-temperature mass spectrometry. A mass spectrometric study of the possibility of congruent transition to the gas phase of complexes of octapropylsubstituted porphyrazine complex with silicon difluoride SiF_2Pr_8Pz and ethioporphyrinate-I of silicon difluoride SiF_2EtioP-I was performed. The study was carried out using a magnetic mass spectrometer MI-1201, modified for thermodynamic studies. The enthalpies of sublimation of SiF_2Pr_8Pz and SiF_2EtioP-I were determined using the Knudsen effusion method with mass spectrometric control of the composition of the gas phase. In the case of SiF_2Pr_8Pz, the vapor pressure and entropy of sublimation were determined. The enthalpies of sublimation determined based on the temperature dependences of the molecular ions intensities using the Clausius-Clapeyron equation were found to be 191(4) and 235(5) kJ/mol for SiF_2Pr_8Pz and SiF_2EtioP-I in the temperature ranges 523-566 K and 481-544 K, respectively. The values of the entropy of sublimation for SiF_2Pr_8Pz and SiF_2EtioP-I were 293(2) and 392(3) J/(mol*K), respectively. Cobalt(II) hemiporphyrazine (CoHp) is also one of the objects of our thermodynamic research. The enthalpy of sublimation for CoHp is 212(5) kJ/mol in the temperature range of 481–544 K.

The gas-phase molecular structure of SiF_2EtioP-I have been studied by a synchronous gas-phase electron diffraction and mass spectrometric experiment and DFT calculations. Electron diffraction studies are of particular importance because the obtained molecular structure is free from collective interactions characteristic of X-ray and neutron diffraction. This allows for highly reliable determination of fine details of the molecular geometry.

An important component of this research is the theoretical determination of the geometric and electronic structure of macrocycles using quantum-chemical calculations, which made it possible to determine the influence of substituents on the structure and spectral properties of these compounds. Quantum-chemical calculations for a number of complexes with macroheterocyclic ligands were performed: porphyrazine complexes with silicon(IV), germanium(IV), tin(IV) and lead(IV) $XPzY_2$ (X = Si, Ge, Sn, Pb; Y = F, Cl, Br, OH), the octa(4-propylphenoxy)phthalocyanine complexes with Al(III), Ga(III) and In(III).

The structure of free molecules, possibility of congruent phase transition of macroheterocyclic compounds into the gas phase, their thermal stability, as well as the vapor composition and enthalpy of sublimation will certainly be useful in developing the technical processes of resistive evaporation in vacuum of these substances.

This work was supported by RSF (project № 24-73-10107).

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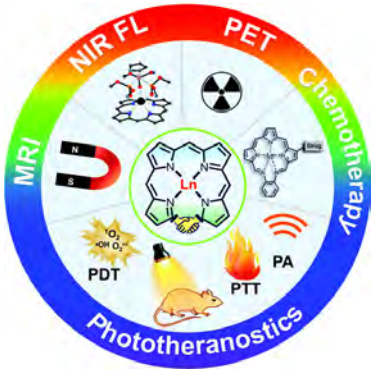
NIR Lanthanide Phototheranostics

Jun-Long Zhang[a]

[a] *Beijing National Laboratory for Molecular Sciences, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P. R. China*

ORALS

From a chemist's perspective, theranostics represents an emerging paradigm that relies on the design of targeted agents capable of integrating diagnostic and therapeutic functions within a single platform.[1] As such, it offers an attractive strategy for addressing key challenges in the development of next-generation personalized medicine. In recent years, lanthanide (Ln) porphyrinoids have attracted growing interest as versatile theranostic agents.[2] This talk will discuss their applications in near-infrared (NIR, 650–1700 nm) fluorescence imaging (FL), magnetic resonance imaging (MRI), radiotherapy, and chemotherapy.[3] Particular emphasis will be placed on the use of Ln porphyrinoids as photoactivated agents ("phototheranostics"), highlighting three promising strategies for regulating porphyrinic triplet energy dissipation pathways: regioisomeric effects, metal-centered regulation, and the use of expanded porphyrinoids.[4] Overall, this presentation aims to showcase ongoing efforts to optimize Ln porphyrinoids for theranostic and phototheranostic applications, while providing insight into future directions in the field, including structure-driven innovation, enhanced functional performance, and emerging biologically activated strategies.



Scheme 1. Schematic diagram of Ln porphyrinoid theranostics (copyright from **Chem. Soc. Rev.**, 2022,**51**, 6177-6209)

REFERENCES (05_REFERENCES_TITLE)

1. J. Funkhouser *Curr. Drug Discovery*, 2002, **2** , 17-19 ;
2. G.-Q. Jin, C. V. Chau, J. F. Arambula, S. Gao, J. L. Sessler and J.-L. Zhang, *Chem. Soc. Rev.*, 2022, **51**, 6177-6209;
3. M. Zhu , H. Zhang , G. Ran , D. N. Mangel , Y. Yao , R. Zhang , J. Tan , W. Zhang , J. Song , J. L. Sessler and J.-L. Zhang , *J. Am. Chem. Soc.*, 2021, **143** , 7541 —7552
4. G.-Q. Jin , H. Lai , Z.-S. Yang , Y. Ning , L. Duan , J. Zhang , T. Chen , S. Gao and J.-L. Zhang , *Chem. – Asian J.*, 2022, **17** , e2022001

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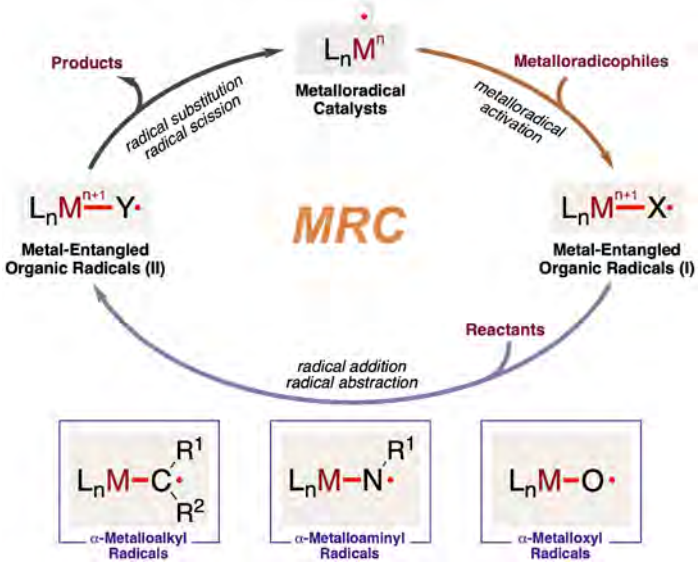


Open-Shell Metalloporphyrins as Metalloradical Catalysts for Homolytic Radical Reactions

X. Peter Zhang[a]

[a]*Department of Chemistry, Boston College, Chestnut Hill, MA 02467-3860, USA*

Organic synthesis has predominantly relied on developing chemical reactions based on two-electron heterolytic ionic processes. While one-electron homolytic radical chemistry is equally rich and exhibits unique features, its application to the stereoselective synthesis of organic molecules has been hindered by persistent challenges. Over the past two decades, my laboratory has been dedicated to formulating metalloradical catalysis (MRC) as a general concept to guide the development of innovative approaches to control both reactivity and stereoselectivity in radical reactions. MRC harnesses the potential of metal-centered radicals in metalloradical complexes as one-electron catalysts for the homolytic activation of substrates, generating metal-entangled organic radicals as key intermediates that direct the reaction pathway and influence the stereochemical outcomes of subsequent catalytic radical processes. To achieve enantioselective radical reactions via MRC, we have introduced a unique family of chiral metalloradical catalysts based on structurally well-defined open-shell metal complexes of D_2-symmetric chiral porphyrins, such as Co(II) and Fe(III) complexes. These chiral metalloradical catalysts offer tunable electronic, steric, and chiral environments. They have demonstrated exceptional efficacy in a wide range of stereoselective organic reactions, including olefin cyclopropanation, olefin aziridination, C–H alkylation, and C–H amination. The Co(II)- and Fe(III)-based MRC exhibits distinctive stepwise radical mechanisms involving α-metalloalkyl and α-metalloaminyl radicals as key intermediates. These metalloradical systems not only address long-standing challenges in these important organic transformations but also provide ample opportunity for the development of new synthetic tools.



ORALS

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Porphyrin nanomedicine: from activatable photosensitizers to radiopharmaceuticals

Gang Zheng[a,b]

[a]*Department of Medical Biophysics, University of Toronto*
[b]*Princess Margaret Cancer Centre, University Health Network*

ORALS

Activatable photosensitizers are a class of photodynamic therapy (PDT) agents engineered to "turn on" in response to disease-specific biostimuli, thereby improving therapeutic selectivity and minimizing off-target effects [1]. In the search for a nanoparticle-based activatable photosensitizer, we developed porphysomes [2], liposome-like nanoparticles self-assembled from a single porphyrin–lipid building block. Their unique structure renders them photothermal and photoacoustic when intact, and fluorescent and photodynamically active upon disruption. Beyond their optical properties, direct chelation of radionuclides within the porphyrin macrocycle enables porphysomes to serve as versatile nuclear medicine agents [3]. We have demonstrated that ^{64}Cu and ^{67}Cu can be stably incorporated into porphysomes, enabling PET or SPECT imaging and laying the foundation for radionuclide therapy.

We advanced this platform from conceptual design to preclinical maturity, leveraging academic infrastructure to satisfy regulatory requirements and perform comprehensive validation in cancer models [4]. A first-in-human clinical trial using ^{64}Cu-porphysomes for metastatic ovarian cancer is now underway (NCT06977126), with the first patient already safely dosed. To further broaden the radiometal chelation capabilities of porphysomes, we developed next-generation nanoparticles composed of texaphyrin–lipid building blocks. These "nanotexaphyrins" stably chelate a wide range of metals—including Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Tl, Mn, Fe, Co, Y, Cd, In, Re, Pb, and Bi—substantially expanding the radiotheranostic potential of the porphysome platform [5].

REFERENCES

1. Kwon N *et al*, Activatable Photosensitizers: from Fundamental Principles to Advanced Designs, *Angewandte Chemie* 2025, 64, e202423348.
2. Lovell *et al*, Porphysome Nanovesicles Generated by Porphyrin Bilayers for use as multimodal biophotonic contrast agents, *Nature Materials* 2011, 10: 324-332.
3. Liu *et al*, Intrinsically copper-64-labeled organic nanoparticles as radiotracers. *Angewandte Chemie* 2012, 51: 13128-31.
4. Valic *et al*, Radiopharmaceutical kit to prepare Copper-64 labelled porphyrin-lipid nanoparticles for radiotracer imaging studies in cancer patients, *Eur J Nucl Med Mol Imaging* 2025, 10.1007/s00259-025-07442-5.
5. Cheng *et al*, Targeted Theranostic ^{111}In/Lu-Nanotexaphyrin for SPECT Imaging and Photodynamic Therapy. *Mol Pharm*, 2022, 19, 1803–1813.

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Interrogating Electronic Structure in N-Confused Porphyrins

Christopher J. Ziegler

Department of Chemistry, Unviersity of Akron, Akron OH USA44321

For more than a quarter of a century, the chemistry N-confused porphyrin (NCP) has fascinated the chemistry community. NCP is an isomer of normal porphyrin with a single inverted pyrrole ring that has the same steric footprint as normal porphyrin. However, this small change produces a porphyrinoid that exhibits notable differences form normal porphyrin, which can be seen in its metalation chemistry, tautomerization behavoir, stability, and spectroscopic properties. In this presentation, we will present our work on using spectroscopy and computations to elucidate the electronic structure of N-confused porphyrins and their metal complexes. The swapping of two atom positions in the porphyrin skeleton produces a macrocycle with significant alterations to its frontier four orbital electronic structure. In many cases, we observe an inverstion of the normal ΔHOMO > ΔLUMO relationship, which can often be reversed via deprotonation or tautomerization changes.

REFERENCES

1. Inorg. Chem. 2011, 50, 15, 6902–6909.
2. J. Phys. Chem. A 2013, 117, 45, 11499–11508.
3. J. Phys. Chem. Lett. 2023, 14, 33, 7382–7388.

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Assessment of cationic phthalocyanines and doxycycline against resistant microbes – innovative approach or dead end?

Daniel Zientala, Jolanta Dlugaszewskab, Eduardo Anaya Plazac, Andrés de la Escosurad, Tomas Torresd, Ana Belen Domínguezd, M. Salome Rodríguez-Morgaded Lukasz Sobottaa

[a] *Chair and Department of Inorganic and Analytical Chemistry, Poznan University of Medical Sciences, Rokietnicka 3, 60-806 Poznan, Poland*
[b] Chair and Department of Genetics and Pharmaceutical Microbiology, Poznan University of Medical Sciences, Rokietnicka 3, 60-806 Poznan
[c] Department of Bioproducts and Biosystems, School of Chemical Engineering, Aalto University. Kemistintie 1, 00076 Aalto, Finland.
[d] Departamento de Química Orgánica (C-I) and Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid, Spain

Two sets of phthalocyanine-based compounds (PS1a–PS4a and 1–5), developed at the Autonomous University of Madrid, were evaluated for their photodynamic activity against multidrug-resistant pathogens. The Ru(II) complexes PS1a–PS4a, bearing multiple ammonium groups and displaying high singlet oxygen yields, showed strong activity against MRSA and *E. coli* under low light doses. Their ability to penetrate and bind to cell wall and membrane structures was confirmed, with amphiphilic derivatives (PS3a, PS4a) designed for enhanced intracellular targeting. Notably, PS4a exhibited synergism with subinhibitory doxycycline, increasing MRSA reduction from 1.5 to 4.9 logs. Compounds 1–5, functionalized with pyridyloxy and bulky hydrophobic substituents, demonstrated broad-spectrum efficacy against S. aureus, MRSA, *E. faecalis*, *E. coli* (including ESBL-producing strains), *P. aeruginosa* (including carbapenem-resistant), *C. albicans*, and *T. mentagrophytes*, achieving reductions of 1.4–5.6 logs. Several derivatives also showed enhanced antimicrobial effects in combination with doxycycline. These results highlight the therapeutic potential of cationic
phthalocyanines in photodynamic control of resistant pathogens.

REFERENCES

[1] Ziental D, Plaza EA, Talarska-Kulczyk P, Kubicka A, Żurawski J, Dlugaszewska J, et al. Quaternized phthalocyanines as a tool against melanoma and a broad spectrum of bacteria and fungi. Journal of Photochemistry and Photobiology B: Biology. 2025 May 28;113187.
[2] Domínguez AB, Ziental D, Dlugaszewska J, Sobotta L, Torres T, Rodríguez-Morgade MS. Multicationic ruthenium phthalocyanines as photosensitizers for photodynamic inactivation of multiresistant microbes. European Journal of Medicinal Chemistry. 2025 Mar 5;285:117214.

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New Near-Infrared Photoimmunotherapeutic (NIR-PIT) Drugs for Anti-Cancer Treatment

Saswati Adhikary[a], Akari Mukaimine[a], Mikako Ogawa[a,b]

[a]*WPI-ICReDD, Hokkaido University, Sapporo, Japan;*
[b]*Laboratory of Bioanalysis and Molecular Imaging, Graduate School of Pharmaceutical Sciences, Hokkaido University, Sapporo, Japan*

Cancer treatment using antibody–IR700 is part of the near-infrared photoimmunotherapy (NIR-PIT) method, which induces immunogenic cell death in cancer cells upon NIR light. It was approved in Japan in 2020 for the treatment of head and neck cancer, and a global phase II trial is currently underway. Combining NIR-PIT with various anticancer drugs may enhance effectiveness, depending on the tumor microenvironment (TME).

To inhibit cancer growth, the efficacy of proteins (EGRF, VEGRF) needs to be inhibited in TME. So, IR700 conjugated afatinib (EGFR) and sunitinib (VEGFR) have been developed. Drug releasing efficacy from the IR700-drug conjugate upon NIR light irradiation has been performed. [Protocol: IR700-drug conjugates: 5 μM in phosphate buffer (10 mM, pH 7.0) with 1 mM L-cysteine. This solution was degassed by Agon gas for 20 minutes, followed by a NIR light dose. Analysis was then performed using HPLC before and after each NIR light dose (Figure 1).

Several types of IR700-drug conjugates have been successfully synthesized. NIR irradiation experiment has been performed, which indicates IR700 and afatinib or sunitinib have been released in a dose-dependent manner. Currently, in-vitro studies are ongoing to assess the anticancer efficacy of IR700-drug conjugate using human cancer cells. The aim of this study is to combine NIR-PIT with various anticancer drugs to enhance effectiveness, depending on the TME.

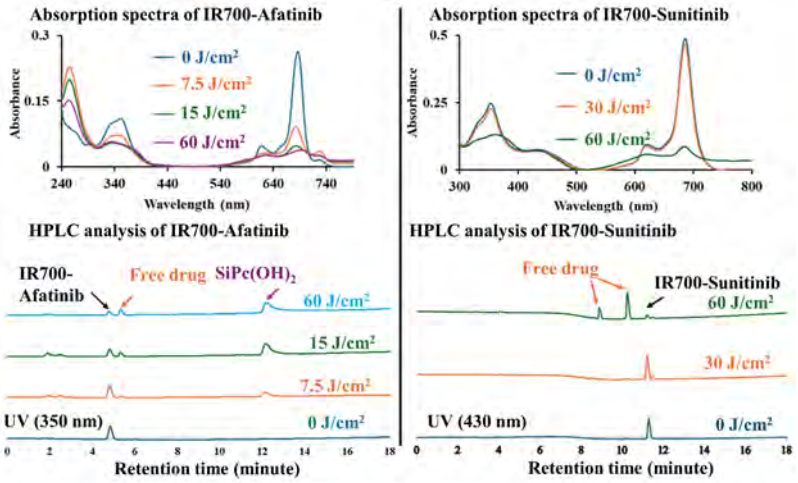


Figure 1: NIR-irradiation experiment of IR700-Afatinib and IR-Sunitinib conjugate.

REFERENCES

1. Mitsunaga M, et al., *Nat. Med.* 17(12), 1685-1691 (2011).

POSTERS

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From Aromaticity to Catalysis: Symmetry-Driven Electronic Structure Modulation in Functional Macrocycles

Md Ashif Ali[a], Woo-Dong Jang[b*] and Dongho Kim[c*]

[a]*Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Korea, E-mail: alimd5283@yonsei.ac.kr*

[b]*Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Korea, E-mail: wdjang@yonsei.ac.kr*

[c]*Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Korea, E-mail: dongho@yonsei.ac.kr*

π-Conjugated macrocycles represent fundamental architectures in chemistry due to their tunable aromaticity [1], rich electronic structures, and diverse functional applications [2]. Despite extensive studies on porphyrinoids and expanded macrocycles, a unified understanding of how symmetry breaking modulates electronic structure and translates into functional outcomes—particularly in the context of excited-state aromaticity and catalysis—remains limited. In this work, we investigate symmetry-driven electronic structure modulation in expanded and metalated macrocycles. N-fused bridged asymmetric 36π octaphyrins are employed to examine the impact of reduced symmetry on ground- and excited-state aromatic characteristics, including Baird aromaticity [3], revealing distinct delocalization pathways arising from structural perturbation. In parallel, triazole based iron (III) porphyrin systems are explored in carbene transfer catalysis, where atropisomeric differentiation [4] and secondary coordination sphere effects lead to measurable variations in cyclopropanation efficiency. Combined experimental and computational analyses demonstrate that symmetry reduction induces electronic redistribution that governs both aromatic behaviour and catalytic reactivity. This study establishes clear structure–symmetry–reactivity relationships in π-conjugated macrocycles and provides mechanistic insight for the rational design of functional macrocyclic systems.

REFERENCES

1. J. Kim, J. Oh, A. Osuka and D. Kim, *Chem. Soc. Rev.*, 2022, **51**, 268–292.
2. C. Damiano, P. Sonzini and E. Gallo, *Chem. Soc. Rev.*, 2020, **49**, 4867–4905.
3. N. C. Baird, *J. Am. Chem. Soc.*, 1972, **94**, 4941–4948.
4. D. J. Martin, B. Q. Mercado and J. M. Mayer, *Inorg. Chem.*, 2021, **60**, 5240–5251.

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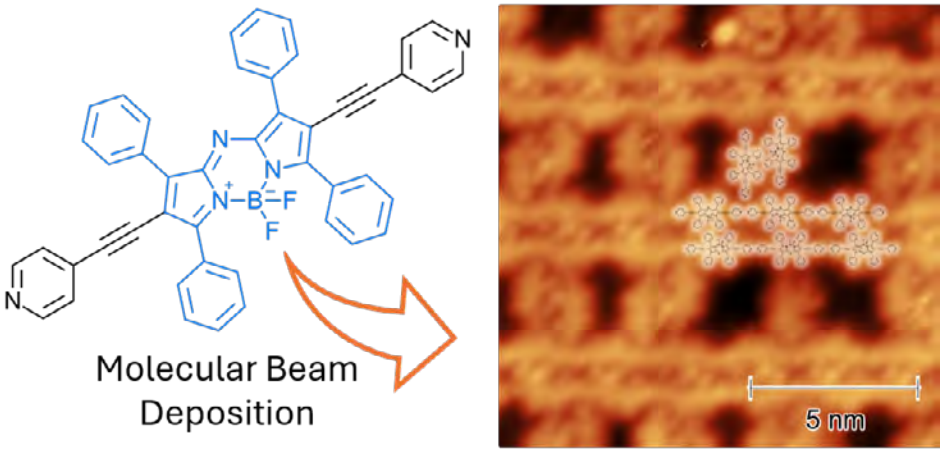


Towards On-Surface Photoswitching of Electronic Conductivity with Aza-BODIPY Molecular Wires

Yannic Altmann[a,b], René Matzdorf[b], Rüdiger Faust[a]

[a]*University of Kassel, Institute for Chemistry and CINSaT, Heinrich-Plett-Str. 40, 34132 Kassel, Germany, r.faust@uni-kassel.de*
[b]*University of Kassel, Institute for Physics and CINSaT, Heinrich-Plett-Str. 40, 34132 Kassel, Germany*

The concept of conductance switching is an integral part of molecular electronics. Of particular interest is the concept of light-responsive molecular switching which can either be achieved by light-induced configurational or conformational changes or by addressing conductivity differences between the ground and the excited states of photoconducting molecules. [1-3] We became interested in the surface deposition of semiconducting aza-BODIPYs, a class of molecules that feature intense electronic absorptions in the visible region [4] and have initiated a programme to explore their single-molecule conductance on solid surfaces. In particular, we aim to identify differences in the conductivity of these molecules upon photoexcitation on surface.
In our current work, we report the synthesis of pyridylethynyl-functionalized aza-BODIPY molecules designed to enable anchoring to common metallic electrode materials via the pyridine-nitrogen and a conductance path across the π-electron perimeter. In addition, we report the single-layer deposition, the self-assembly of the aza-BODIPY molecular wires on the Au(111) surface and we will present initial results on conductivity measurements using scanning tunnelling microscopy break junctions (STM-BJ).



REFERENCES

1. X. Xu, C. Gao, R. Emusani, C. Jia, D. Xiang, *Adv. Sci.* **2024**, 11, 2400877.
2. M. Galperin, A. Nitzan, *Phys. Chem. Chem. Phys.* **2012**, 14, 9421-9438
3. J. Zhou, K. Wang, B. Xu, Y. Dubi, *J. Am. Chem. Soc.* **2018**, 140, 70–73
4. J. Meyer, A. Wadewitz, Lokamani, C. Toher, R. Gresser, K. Leo, M. Riede, F. Moresco and G. Cuniberti, *Phys. Chem. Chem. Phys.* **2011**, 13, 14421-14426

POSTERS

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Light-induced molecular motion in supramolecular fibres

Daniela Dupkalová,[a] Aysha Fasna,[ab] David B. Amabilino,[b] Monika Gupta[c] and Lluïsa Pérez-García[a]

[a] *Departament de Farmacologia, Toxicologia i Química Terapèutica, Universitat de Barcelona, Av. Joan XXIII 27-31, Barcelona, 08028, Spain and Institut de Nanociència i Nanotecnologia UB (IN2UB)*
[b] *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Carrer del Til.lers, 08193 Bellaterra, Spain*
[c] *Department of Chemistry, Indian Institute of Technology Jodhpur, Rajasthan, 342030, India*

Various synthetic stimuli-responsive microscopic systems with impressive control in relative molecular motion have been created [1] to imitate naturally occurring movement of biomolecules. Our group developed a purely supramolecular system where a molecular 'traveller' (**TCPP**) moved along gemini bis-imidazolium gelator fibers over several microns when irradiated with visible light in the presence of photoswitch (**Azo**) [2].
In this work, we present a modified system with different azobenzene derivative (**AzoF4**) incorporated as a photoswitch (Figure). Because of higher *cis*:*trans* ratio, **AzoF4** could change the extent of observed **TCPP** movement. Moreover, *cis*-isomer population can be easily replenished using visible light, allowing repeated energy release. Real-time imaging of the motion in the solvated state was recorded using total internal reflection fluorescence (TIRF) microscopy.

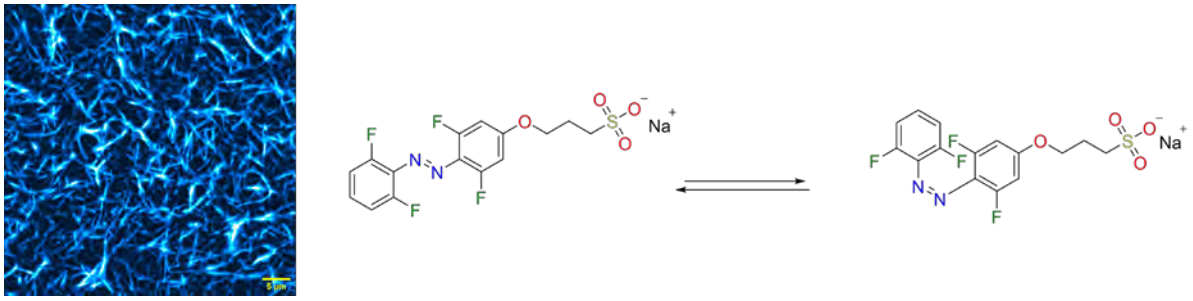


Figure: a) TIRF microscopy image of hydrogel with **AzoF4** and **TCPP** incorporated in the fibers. b) Molecular structure of **AzoF4** in *trans* and *cis* state.

Acknowledgments
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REFERENCES

1. Baroncini, M; Silvi, S; Credi, A. "Photo- and Redox-Driven Artificial Molecular Motors," *Chem. Rev*. **2020**, *120*, 200.
2. Samperi, M.; Bdiri, B.; Sleet, C. D.; Markus, R.; Mallia, A. R.; Pérez-García, L.; Amabilino, D. B. "Light-controlled micron-scale molecular motion," *Nat. Chem.,* **2021**, *13*, 1200.

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Electrochemical generation of reactive Nitrido complexes for Nitrogen Atom Transfer

Kirill Kuznetsov Jérémy De Freitas, Marc Robert, Claire Fave
Élodie Anxolabéhère-Mallart,

Institut Parisien de Chimie Moléculaire UMR 8232, Sorbonne Université, 4 Place Jussieu, 75252 Paris Cedex 05, France

The activation of small molecules, such as H_2, CO_2, O_2, N_2, and NH_3, is of fundamental importance in chemistry, particularly for the development of new and sustainable synthetic processes. However, the activation of these molecules remains challenging due to their high chemical stability and inertia. In this context, the combined use of electrochemistry and inexpensive, earth-abundant molecular catalysts based on manganese represents a promising and sustainable strategy.[1–4] The global ammonia production is expected to increase by approximately 40% by 2050, thus, the development of new approaches that exploit ammonia as a nitrogen source is particularly relevant. In a preliminary study, our team demonstrates the electrochemical oxidation of ammonia to dinitrogen under homogeneous conditions, catalyzed by complex Mn^{III}(TPP)(Cl). Preparative-scale electrolysis of Mn^{III}(TPP)(Cl) with NH_3 at +1.42 V vs. SCE resulted in one of the highest Faradaic efficiencies of 100% and turnover number (TON = 12). This high level of nitrogen activation motivated us to explore the reactivity of this system and, in particular, to study the functionalization of C–H and C–C π-bonds via nitrogen atom transfer. In the present work, we study Mn^{III}(TPP)(Cl) porphyrin as a catalyst and styrene as a substrate for the production of aziridine derivatives. Based on the results, we were able to propose a possible mechanism for the anticipated catalytic cycle (Figure 1).

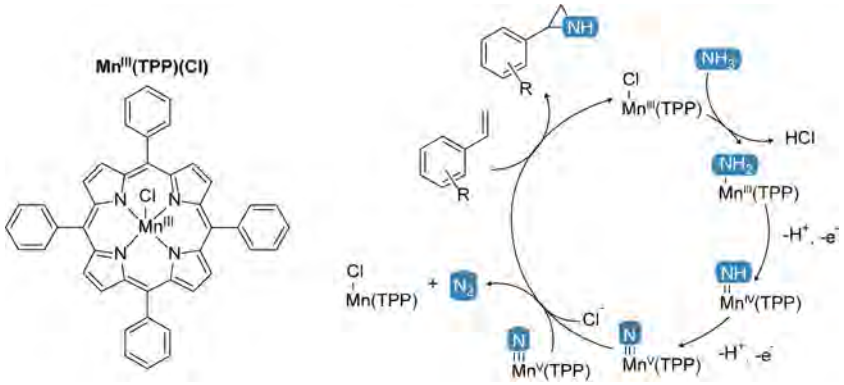


Fig. 1. *Mn^{III}(TPP)(Cl) (left) and proposed mechanism of catalytic cycle (right).*

REFERENCES

1. R. M. Clarke and T. Storr, *J. Am. Chem. Soc.*, 2016, **138**, 15299–15302.
2. H. Shi, H. K. Lee, Y. Pan, K.-C. Lau, S.-M. Yiu, W. W. Y. Lam, W.-L. Man and T.-C. Lau, *J. Am. Chem. Soc.*, 2021, **143**, 15863–15872.
3. H. Shi, R. Liang, D. L. Phillips, H. K. Lee, W.-L. Man, K.-C. Lau, S.-M. Yiu and T.-C. Lau, *J. Am. Chem. Soc.*, 2022, **144**, 7588–7593.
4. J. Xiang, H. Shi, W.-L. Man and T.-C. Lau, *Acc. Chem. Res.*, 2024, **57**, 2700–2716.

POSTERS

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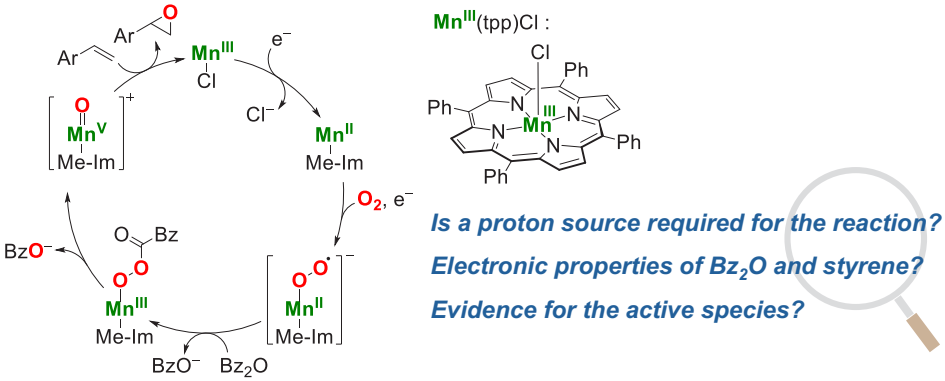


Mechanistic Investigation on the Oxygen Atom Transfer to Styrene *via* the Electrochemical O_2 Activation by a Mn-Porphyrin

Sara I. Mozzi, Ireneusz Tomczyk, Sihem Groni, Sittichok Kasemthaveechok, Claire Fave, Elodie Anxolabéhère-Mallart

Sorbonne Université, Institut Parisien de Chimie Moléculaire UMR 8232, CNRS, 75005 Paris, France

Oxygen atom transfer (OAT) reactions play a key role in the synthesis of relevant chemical feedstock and intermediates in the industrial and pharmaceutical fields.[1] Large scale application of these two-electron oxidation reactions typically requires harsh conditions and the stoichiometric use of high-energy oxidants, which constitute safety hazards.[2] Molecular dioxygen (O_2) represents an appealing readily available alternative as green oxidant, however, its spin-triplet ground state leads to a kinetic inertness towards the reaction with organic substrates. With nature as a blueprint, bioinspired molecular catalysts able to perform OAT *via* the electrochemical reductive activation of O_2 have been developed.[3] Herein, we bring new insights into the pioneering work of Murray[4] on a Mn porphyrin complex as electrocatalyst for the epoxidation of styrene in presence of benzoic anhydride. Diving into the reaction mechanism (Scheme 1), the impact of acid and the electronic properties of *p*-substituted benzoic anhydrides and styrenes are investigated *via* electrochemical methods such as cyclic voltammetry and controlled potential electrolysis. In addition, the Mn-oxo porphyrin cation species responsible for OAT, reminiscent of the mechanism found in nature, is identified.



Scheme 1: Proposed catalytic cycle for the styrene epoxidation by Mn^{III}(TPP)Cl in presence of O_2.

REFERENCES

1. a) J. H. Teles, W. Partenheimer, R. Jira, F. Cavani, G. Strukul, R. Hage, J. W. Boer, L. Gooßen, P. Mamone, O. A. Kholdeeva, *Oxidation in Applied Homogeneous Catalysis with Organometallic Compounds: A Comprehensive Handbook in Four Volumes, Third Edition*, Wiley, **2017**.
2. G. Li, A. K. Dilger, P. T. Cheng, W. R. Ewing, J. T. Groves, *Angew. Chem. Int. Ed.* **2017**, *57*, 1251.
3. a) M. Mukherjee, A. Dey *ACS Cent. Sci.* **2019**, *5*, 671−682. b) E. Anxolabéhère-Mallart, F. Banse, *Curr. Opin. Electrochem.* **2019**, *15*, 118. c) N. Kostopoulos, F. Banse, C. Fave, E. Anxolabéhère-Mallart, *Chem Commun* **2021**, *57*, 1198.
4. S. E. Creager, S. A. Raybuck, and R.W.Murray, *JACS*, **1986**, *108*, 4225-4227.

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Prevention of pneumonia with functionalized endotracheal tubes and antimicrobial photodynamic therapy

L. G. Arnaut[a,b], Carlos Serpa[a,b], Fábio M. S. Rodrigues[a], Amanda Rocha[c], Kate C. Blanco[c], Anderson Zanchin[d], Mariette M. Pereira[a], Vanderlei S. Bagnato[c]

[a] *Chemistry Department, University of Coimbra, Coimbra, Portugal*
[b] *LaserLeap Technologies SA, Rua Col. Júlio Veiga Simão, S/N CTCV, Edifício B, 3025- 307 Coimbra, Portugal*
[c] *Instituto de Física de São Carlos – Universidade de São Paulo, São Carlos – SP, 13566-590, Brasil*
[d] *MMOptics Ltda, Rua Geminiano Costa, 143 – São Carlos, SP, 13560-641, Brasil*

A major health problem of the post-antibiotic era is the surge in hospital-acquired (nosocomial) infections, which affect 3.2% and 6.5% of hospitalized patients in the USA and in the European Union, respectively. Ventilator-associated pneumonia (VAP), catheter-associated urinary tract infections, and central-catheter bloodstream infections represent ~25% of nosocomial infections. We showed that the functionalization of PVC surfaces of endotracheal tubes (ETTs) with photosensitizers and their regular illumination prevents colonization by *S. aureus*, *E. coli* and *P. aeruginosa* [1]. Subsequently, comparable results can be obtained in the prevention of fungal spread, such as *Candida* [2]. Here, we report *in vivo* studies designed to assess the prevention of biofilm formation in ETTs entubated in pigs for 24 h or 72 h. Three animals were included in the 24 h control group, which were intubated with commercial ETTs (not functionalized). Five animals were included in the 24 h treatment group, in which the animals were intubated with functionalized ETTs and illuminated at 2 h, 6 h, 18 h, and 22 h post-intubation. The total light dose was 400 J/cm^2. The 8 pigs intubated for 24 h under mechanical ventilation remained with stable vital data for 24 hours, but only one pig in each of the 72 h control and treatment groups could be evaluated at the end of the experiment. At the end of the experiments, the ETTs were collected and analyzed regarding bacterial colonization. The lumen of the ETTs in the treatment group presented a significantly lower bacterial load than that of the commercial ETT. Analysis of the lung parenchyma after 24 h revealed a lower bacterial load than in the oral cavity and trachea, and lower in the treatment group than in the control group. OCT analysis of the ETTs in the 72 h experiments conclusively showed that the control ETT hosted a biofilm, but the treatment group ETT was as clean as pristive ETTs. Functionalization of ETTs with photosensitizers, followed by antimicrobial PDT, significantly reduces colonization of the tubes and lungs. Current experiments explore the functionalization of ETTs with a variety of photosensitizers, which share the common goal of establishing a covalent bond between the photosensitizer and the surface of PVC tubes.

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REFERENCES

1. A. C. Zangirolami, L. D. Dias, K. C. Blanco, C. S. Vinagreiro, N. M. Inada, L. G. Arnaut, M. M. Pereira, V. S. Bagnato, *Proc. Natl. Acad. Sci. USA*, 117 (2020) 22967-22973. DOI: 10.1073/pnas.2006759117.
2. G. G. dos Santos, A. C. Zangirolami, M. L. F. Vicente, V. S. Bagnato, K. C. Blanco. Photodynamic therapy as a potential approach for preventing fungal spread associated with the use of endotracheal tubes. *Photochem Photobiol* 101 (2025) 858-868 DOI: 10.1111/php.14054
3. A. C. Zangirolami, V. S. Bagnato, L. D. Dias, N. M. Inada, C. S. Vinagreiro, L. G. Arnaut Moreira, M. M. Pereira, K. C. Blanco. Method for obtaining functionalized polymeric surfaces with photosensitizers, functionalized polymeric materials and use thereof. WO2021/007638A1, 21/01/2021. PCT/BR2020/050263.

POSTERS

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Optical characterisation of single chlorophyll molecules at the sub-nanometre scale

Thiago G. L. Brito*[a], Daniel Arribas*[a], Myriam Wadsack[a], Claudia Leticia Gómez Flores[a], Irena Padniuk[a], Victor Feitosa[a,b], Klaus Kuhnke[a], Klaus Kern[a,c], Kelvin Anggara[a], Anna Rosławska[a]

*Equally contributing authors

[a]*Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany*
[b]*University of Campinas - UNICAMP, Campinas 13083-859, Brazil*
[c]*École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland*

As one of the main biomolecules harvesting light in photosynthetic organisms, chlorophyll plays a crucial role in biological systems, ultimately sustaining life on Earth. Therefore, the fundamental understanding of the optical properties of this porphyrin-related biomolecule has attracted widespread interest from the scientific community. However, traditional spectroscopic experiments, often probing complexes, only provide an averaged understanding of the rich photophysics of chlorophyll, where the effects of each possible molecular configuration and the local environment are smeared out. In this work, we address this by exploiting the sub-nm resolution of scanning tunnelling microscopy and the highly-localised plasmonic enhancement of the picocavity at the tunnelling junction. We characterise individual chlorophyll molecules, deposited by electrospray ion beam deposition on a Ag(111) surface with NaCl islands as decoupling layer. By analysing their fluorescence emission excited by the tunnelling electrons or an external laser source and their tip-enhanced Raman spectra, we observe the structural dependency of the molecular opto-electronic properties. Our investigation opens new opportunities for the fundamental understanding of light-harvesting during photosynthesis with unprecedented sub-molecular resolution.

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Alkyl-phthalocyanine based liquid electret

Kodai Asakuma[a,b], **Takashi Nakanishi**[b]

[a]*Chuo University, Tokyo, Japan*
[b]*Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Tsukuba, Japan*

With the rapid expansion of the Internet of Things (IoT), vibration energy harvesters utilizing liquid electrets—which offer ultimate flexibility—are highly anticipated as autonomous power sources and displacement sensors for highly deformable and wearable devices [1-3]. This study aims to develop high-performance liquid electrets and reports the rational molecular design, synthesis, and physicochemical characterization of solvent-free "alkyl-π liquids" at room temperature. The alkyl-π liquids are designed by combining a π-conjugated core, which provides high electrostatic charge retention, with bulky yet flexible branched alkyl chains that not only protect the π-conjugated unit from the environment but also enable it to liquidify at room temperature due to their high entropy.

Specifically, we designed and synthesized novel alkyl-π liquids with a phthalocyanine core, a promising candidate for high-performance liquid electrets, and evaluated their liquid physical properties. Furthermore, the charge amount obtained after corona discharging showed a strong correlation with the electronic structure parameters of the π-conjugated molecules.

During the presentation, we will discuss the aggregation state of the phthalocyanine moieties in liquid, based on optical and viscoelasticity measurements, as well as performance results from a stretchable electret vibration sensor.

POSTERS

REFERENCES

1. Ghosh, A.; Yoshida, M.; Suemori, K.; Isago, H.; Kobayashi, N.; Mizutani, Y.; Kurashige, Y.; Kawamura, I.; Nirei, M.; Yamamuro, O.; Takaya, T.; Iwata, K.; Saeki, A.; Nagura, K.; Ishihara, S.; Nakanishi, T. *Nat. Commun*. **2019**, 10, 4210.
2. Mater. Horiz. Liquid-C60 electrets
3. Angew. Chem. Int. Ed. Alkyl-pi Gel electrets

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Photoactive materials suitable for antimicrobial photodynamic therapy

Stefan Bednarik[a], Dorota Chełminiak-Dudkiewicz[b], Klara Konecna[a], Magdalena Kozlikova[a], Jiri Demuth[a], Petr Zimcik[a], Veronika Novakova[a], Miloslav Machacek[a]

[a] *Faculty of Pharmacy in Hradec Kralove, Charles University, Ak. Heyrovskeho 1203, 500 03 Hradec Kralove, Czech Republic*
[b] *Faculty of Chemistry, Nicolaus Copernicus University in Torun, Gagarina 7, 87-100 Torun, Poland*

Antimicrobial photodynamic therapy (aPDT) has re-emerged as a promising strategy against microbial infections century after the photodynamic effect was first described by Oscar Raab in 1900. [1] Although early development of aPDT was overshadowed by the mid 20th century success of antibiotics, the global rise of antimicrobial resistance has raised an interest in alternative therapeutic approaches. aPDT employs combination of light, oxygen, and a photosensitizer (PS) to generate reactive oxygen species, predominantly singlet oxygen, resulting in targeted oxidative damage to microorganisms. This multi-target mechanism prevents resistance development and enables broad-spectrum antimicrobial activity, including efficacy against antibiotic resistant strains, viruses, and biofilms. Clinical applications are particularly suitable for localized infections due to the spatially confined action of light. PSs represent the core of aPDT, with phenothiazine dyes (such as methylene blue and toluidine blue O) already used clinically in dentistry. [2] However, porphyrinoids, notably phthalocyanines, exhibit superior singlet oxygen generation and potent antimicrobial properties. While cationic PSs are generally more effective, recent findings indicate that molecular symmetry and charge distribution significantly influence antimicrobial performance. This research project aims to develop photodynamically active, biocompatible materials tailored for aPDT with properties that support wound healing. Using complementary experimental approaches, we will design and fabricate materials in multiple formats—including films, sponges, gels, and nanoparticles—constructed from biopolymers, photosensitizers using systems driven by supramolecular interactions or bioorthogonal reactions. The resulting platform is intended to synergistically combine antimicrobial efficacy with promotion of wound-healing, offering a versatile foundation for next-generation aPDT-based therapeutic applications. Upon activation with red visible light, these materials efficiently generate reactive oxygen species, enabling effective eradication of microbial pathogens. This theory was already confirmed using first series of materials containing covalently bound phthalocyanine PSs capable of complete methicillin-resistant *Staphylococcus aureus* (MRSA) eradication after 10 min incubation and irradiation with Xe-lamp equipped with long-pass and water filters ($\lambda > 570$ nm, 22.4 J/cm^2). For *Pseudomonas aeruginosa* and *Candida albicans* only delay in growth was observed – this may not seem like much, but such activities against all strains were not observed for free PSs even at very high concentrations (200 μM). Moreover, these materials have shown negligible toxicity on a 3D model of dermal equivalent composed of normal human fibroblasts embedded in a simulated extracellular matrix. Also, using confocal microscopy, no PSs were detected in human skin incubated with the materials for 24 hours.

Acknowledgments: This work was supported by the Czech Science Foundation grant No. *26-22222K* and and National Science Centre 2025/07/Y/ST5/00057.

REFERENCES

1. O. Raab, *Zeitung Biol* **1900**, *39*, 524–526.
2. Y. Jao, S.-J. Ding, C.-C. Chen, *Journal of Dental Sciences* **2023**, *18*, 1453-1466.

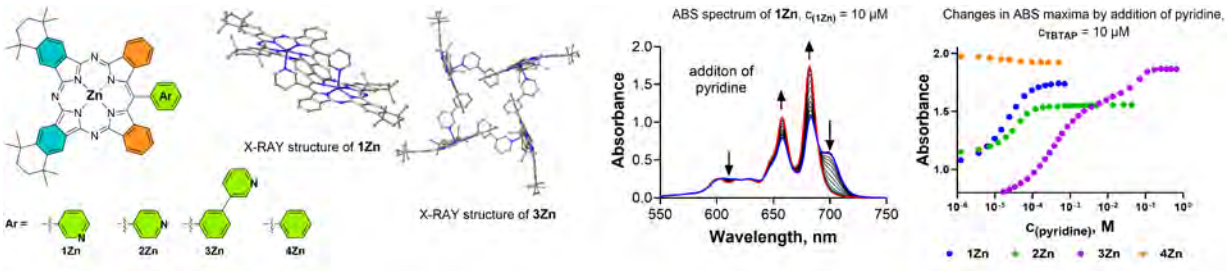
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Self-assembly of *meso*-functionalized ABBA Zinc(II) Tetrabenzotriazaporphyrins into supramolecular systems

Stefan Bednarik[a, b], **Jiri Demuth**[a], **Isabelle Chambrier**[b], **Ales Ruzicka**[c], **Jan Labuta**[d], **Petr Zimcik**[a], **Andrew Cammidge**[b], **Veronika Novakova**[a]

[a] *Faculty of Pharmacy, Charles University, Ak. Heyrovskeho 1203, 500 03 Hradec Kralove, Czech Republic*
[b] *School of Chemistry, Pharmacy and Pharmacology, University of East Anglia, NR4 7TJ, Norwich Research Park, Norwich, United Kingdom*
[c] *Faculty of Chemical Technology, University of Pardubice, Studentska 573, 532 10 Pardubice, Czech Republic*
[d] *Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Ibaraki 305-0044, Tsukuba, Japan*

Phthalocyanines (Pcs) represent a prominent family of aromatic macrocyclic compounds, characterized by an 18-π electron conjugated system. Their structural similarity to porphyrins and their tuneable electronic properties have made them indispensable in fields such as photodynamic therapy or fluorescence sensors. However, H-type aggregation, due to π-π stacking, diminishes these properties by inducing blue-shifted absorption and quenching fluorescence. In contrast, J-type aggregates retain photophysical properties and exhibit red-shifted absorption. [1] Within the broader family of porphinoid systems, hybrid macrocycles such as tetrabenzotriazaporphyrins (TBTAPs) have emerged as structurally intriguing intermediates between Pcs and tetrabenzoporphyrins. TBTAPs are particularly attractive due to their unique *meso*-carbon linkage, which introduces a new functionalization site not present in traditional Pcs. [2] This structural feature enables the incorporation of diverse substituents, allowing for precise modulation of solubility, electronic structure, and self-assembly behavior. This project therefore focuses on the self-assembly behavior of *meso*-pyridyl substituted TBTAP hybrids, aiming to elucidate the structural and environmental parameters that could facilitate J-type aggregation and expand the supramolecular chemistry of functional porphinoid hybrid systems. The position of the nitrogen in N-donor *meso* substituent, and its orientation toward metal of the second molecule controls the final geometry of the assemblies from slipped J-dimers, through linear polymer to distinct tetramer and may be used to finely tune the 3D arrangement. Individual assemblies were characterized by association constants describing the strength of the bond in a given assembly.



The study was supported by Charles University (*GA UK 230723*).

REFERENCES

1. DEMUTH, J., BEDNARIK, S., et al.: *Inorg. Chem. Front.*, 12, **2025**, 1590-1608.
2. ALKORBI, F., CAMMIDGE, A., et al.: *Angew. Chem. Int. Ed.*, 60, **2021**, 7632-7636.

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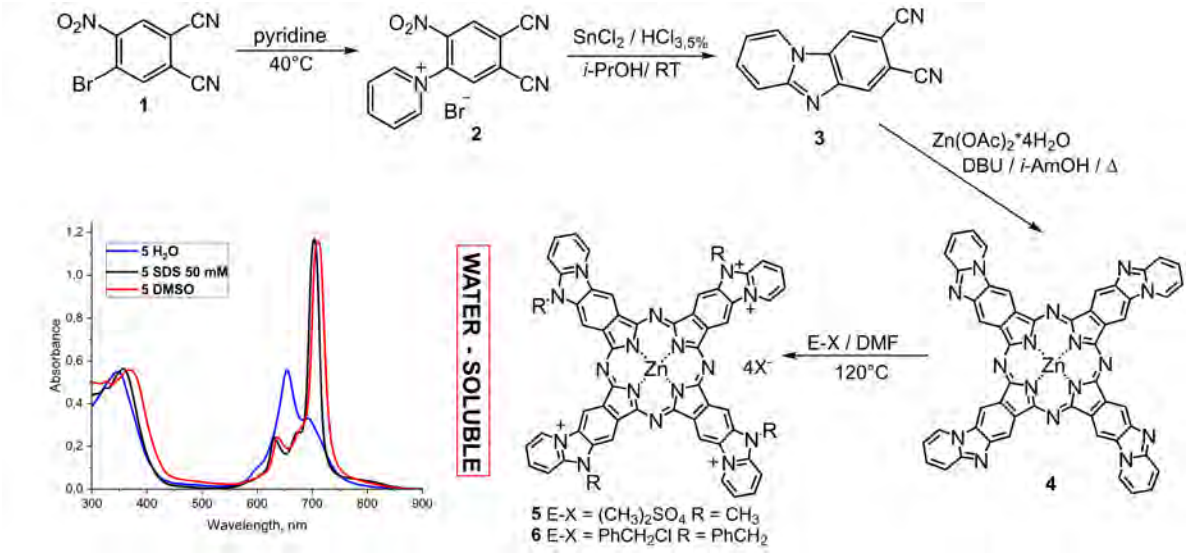


The first pyrido[1,2-*a*]benzimidazole-fused porphyrazines – promising near IR photosensitizers

Mikhail S. Belousov[a], **Ivan D. Burtsev**[b], **Alina A. Markova**[b], **Tatiana V. Dubinina**[a]

[a]*Moscow State University, 1 Leninskie Gory, 119991 Moscow, Russia*
[b]*Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Kosygin st., 4, 119334 Moscow, Russia*

Pyrido[1,2-a]benzimidazole-fused porphyrazines are novel phthalocyanine derivatives in which the porphyrazine core is annelated with four pyrido[1,2-a]benzimidazole moieties. Due to the presence of intense absorption in the near IR region, these compounds are considered as promising photosensitizers for PDT and PACT.
Firstly, pyrido[1,2-a]benzimidazole-fused zinc porphyrazine **4** was prepared using a three-step approach starting from 4-bromo-5-nitrophthalonitrile **1**. The quaternization of this complex was accomplished by reactions with dimethyl sulfate and benzyl chloride electrophiles. This resulted in the preparation of water-soluble cationic photosensitizers **5** and **6**. The aggregation behavior of complexes **5** and **6** in aqueous medium was studied and differential triplet absorption spectra were recorded in DMF. Additionally, the quantum yields of singlet oxygen generation and fluorescence in DMF were measured.
The UV/Vis spectra for the resulting pyrido[1,2-a]benzimidazole-fused porphyrazines show a bathochromic shift of the absorption maximum to the near IR region, up to 746 nm, which is within the range of high transparency of biological tissues. To correctly evaluate the photodynamic efficiency of quaternized complexes, the kinetics of cellular uptake of photosensitizer by malignant cells were studied. Light and dark cytotoxicity were determined on HeLa, HCT116, MCF7, WI38, A549, and A431 cell lines. High photocytotoxicity values reaching IC_{50} = 180 nM were found, with significantly low cytotoxicity values in the dark. As a result, characteristics of the developed photosensitizers were superior to those of chlorin e6, the active component of widely used PDT drugs.



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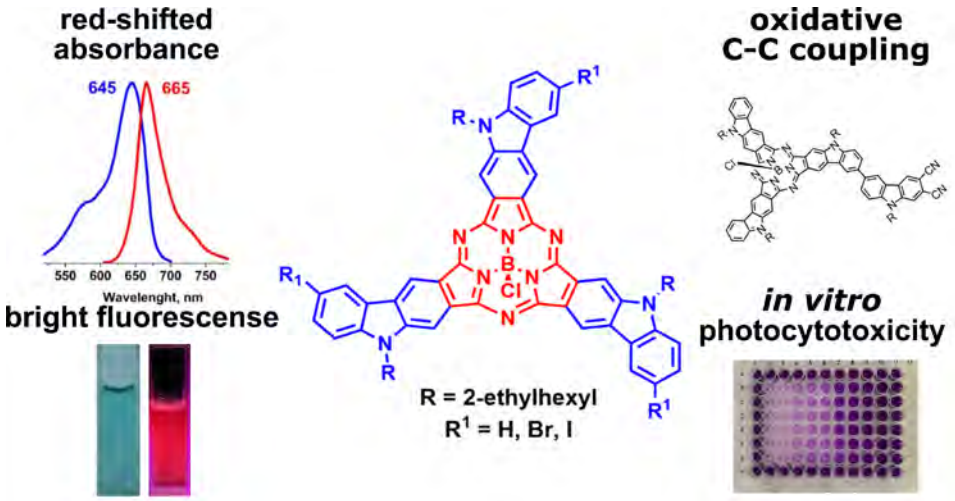
POSTERS

Carbazole-fused boron subporphyrazines: synthesis, photophysical properties and *in vitro* cytotoxicity

Mikhail S. Belousov[a], Maria M. Ivanova[a], Tatiana V. Dubinina[a]

[a]*Moscow State University, 1 Leninskie Gory, 119991 Moscow, Russia*

Due to their non-planar cone-shaped structure, subporphyrazines are not prone to aggregation in solution. Due to high quantum yields of singlet oxygen generation and fluorescence, these compounds can be considered as promising photosensitizers for photodynamic therapy (PDT). However, the absorption maximum of subporphyrazines (*Q* band) is in the range of 500-600 nm, which is outside the high transparency window of biological tissues (600-900 nm). This issue can be addressed by expanding the peripheral π-system of subporphyrazines. In this study, we selected carbazole moieties for attachment to the subporphyrazine core. Initial N-(2-ethylhexyl)-substituted carbazole dinitrile was then prepared by a Suzuki cross-coupling reaction followed by Cadogan cyclization and N-alkylation of the resulting carbazole. Dicyanocarbazole was introduced into the template synthesis in the presence of BCl_3 to obtain the target carbazole-fused subporphyrazine. However, in addition to the target molecule, we observed the formation of poly- and oligomeric byproducts as a result of the oxidative C-C coupling reaction. The introduction of bromine or iodine atoms increases the singlet oxygen quantum yield due to the heavy-atom effect and allows the protection of the 6-position of dicyanocarbazole. For this purpose, dicyanocarbazole was introduced into electrophilic bromination and iodination reactions. Iodinated and brominated dicyanocarbazoles were introduced into the template synthesis, resulting in the corresponding subporphyrazines. It was found that the target complexes have intense absorption in the range of 639-645 nm. In the series of H-Br-I substituents, the singlet oxygen quantum yields increase (0.27, 0.34, 0.42), and the fluorescences yields decrease (0.24, 0.19, 0.17). The possibility of generating a superoxide anion radical was demonstrated. Novel carbazole-containing boron subporphyrazines were found to exhibit micromolar phototoxicity and low cytotoxicity in the dark against the HCT 116 cell line.



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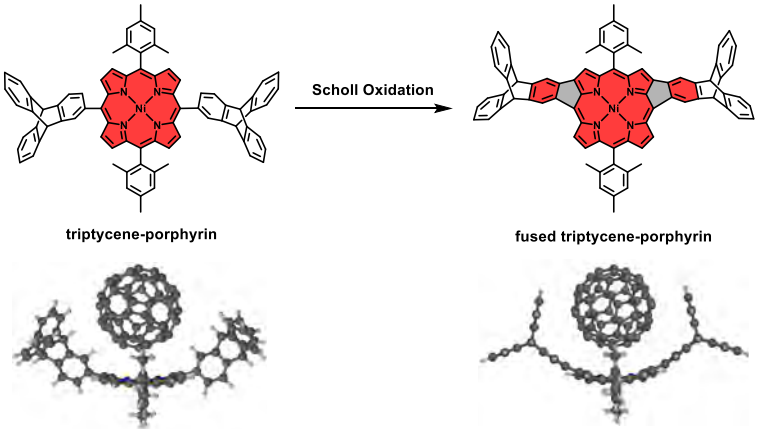


Synthesis of Five-Ring Fused Porphyrins for Supramolecular Chemistry and non-Planar Structures

Benthues Konstantin[a], **Oleszak Christoph**[a], **Ritterhoff Christian**[b], **Jux Norbert**[a]

[a]*Department of Chemistry & Pharmacy and Interdisciplinary Center for Molecular Materials, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nikolaus-Fiebiger Str. 10, 91058 Erlangen, Germany*
[b]*Department of Chemistry & Pharmacy and Interdisciplinary Center for Molecular Materials, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstr. 25, 91052 Erlangen, Germany*

The extension of the aromatic framework of porphyrins has received high attention in the field of organic electronics.[1] As a useful stragedy, Scholl Oxidation of *meso*-aryl porphyrins facilitated a connection to *beta* position of the porphyrin to form a five ring. [2] Post-functionalization led to a drastic change in the photophysical properties of the parent porphyrin. Additionally, using triptycene as arylsubstituent can enhance the properities in supramolecular chemistry.[3] The fused triptycene-porphyrin conjugate may exhibit improved abilities due to the immovable linker arm. This can be demonstrated through computational calculations of host-guest structures with C_{60} fullerene, which reveal a higher-ordered structure of the fused system compared to the non-fused system.



REFERENCES

1. Osuka, *J. et. al. Mater. Chem. C* 2013, *1*, 2500.
2. *Norbert, J. et. al. Eur. J. Org. Chem.* 2020, *2020*, 6758.
3. *Cheng, C. T. et. al. Org. Biomol. Chem.* 2021, *19*, 10047.

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Aza-BODIPY based imaging Biomarkers for anti-cancer applications

Renu Bishnoi[a], Iti Gupta*[a]

[a]Department *of Chemistry, Indian Institute of Technology, Gandhinagar, Palaj, Gandhinagar, 382355, Gujarat, India*

Photodynamic therapy is a non-invasive technique where light, molecular oxygen, and a photosensitizer are used to generate cytotoxic reactive oxygen species for targeted cancer therapy.[1] Among the genrally used photosensitizers, Aza-BODIPY dyes have been used as a promising class of near-infrared (NIR) photosensitizers for photodynamic therapy (PDT). They exhibit strong absorption in the therapeutic window, high molar absorptivity, and excellent photostability which is suitable for PDT. The incorporation of an aza-nitrogen atom into the BODIPY core significantly red-shifts the absorption and emission profiles in NIR region (650–900 nm), enabling deeper tissue penetration and reduced photodamage to healthy tissues.[2] The π-conjugated electrons allow precise modification through peripheral substitution with electron-donating or electron-withdrawing groups or introduction of halogens/heavy atoms to enhance their spectral properties for PDT applications.

Our group at IIT Gandhinagar is involved in the development of sugar linked porphyrins, tin porphyrins and BODIPYs for their applications as photosensitizer against breast cancer.[3-5] In this poster, a new series of functionalized aza-BODIPY will be presented. Their ROS generation and NIR fluorescence properties will be discussed for application in cancer-targeted phototherapy.

POSTERS

REFERENCES

1. Zhao X.; Liu J.; Fan J.; Chao H.; Peng X., *Chem. Soc. Rev.*, **2021**, *50*, 4185-4219.
2. Kaur M.; Janaagal A.; Balsukuri N.; Gupta I., *Coord. Chem. Rev*., **2024**, *498*, 215428.
3. Pandey V.; Raza M.K.; Joshi P.; Gupta I., *J. Org. Chem.*, **2020,** *85*, 6309-6322, **.**
4. Bishnoi R.; Manav N.; Jain A.; Chavda J.; Gupta I., *J. Mol. Struct.,* **2025** *1345*, 143121, .
5. Chavda J.; Siwach A.; Sabharwal S.; Janaagal A.; Bhatia D.; Gupta I.* *ACS Med. Chem. Lett*., **2024,** *15*, 2115-2120.

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Pyrrole-modified *meso*-tetrahexylporphyrin derivatives

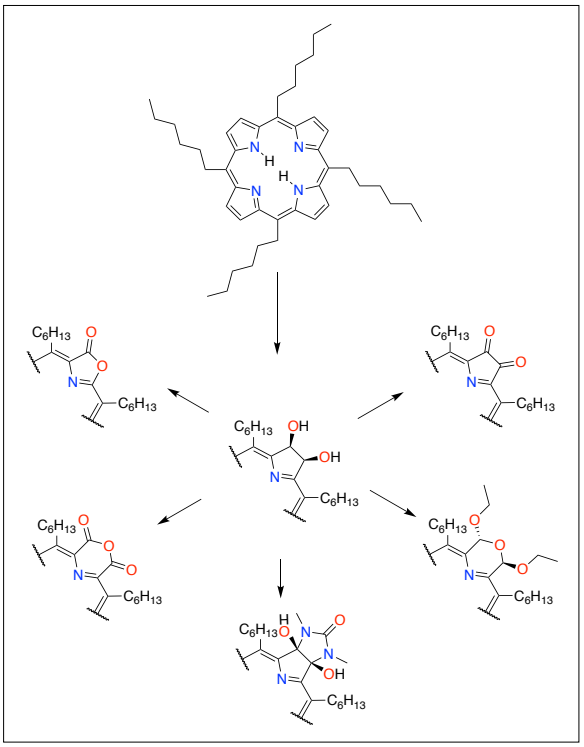
Faith Borkowski and Christian Brückner[a]

[a] *Department of Chemistry, University of Connecticut, Storrs, CT, 06269-3060, U.S.A.*

meso-Tetraarylporphyrins are among the most commonly studied synthetic porphyrins. Over the past decades, we converted tetraarylporphyrins into a variety of so-called pyrrole-modified porphyrins using our "breaking and mending of porphyrins" strategy, typically through modification of a dihydroxychlorin generated by OsO_4-mediated dihydroxylation of the porphyrin [1-2]. In many of these transformations, the *meso*-aryl groups participate directly.

Given their ease of synthesis [3], excellent solubility, and ability to be converted into dihydroxychlorins [4], *meso*-tetraalkylporphyrins have been surprisingly underexplored. Lacking *meso*-aryl substituents, they are expected to exhibit distinct reactivity under some "porphyrin breaking and mending" conditions, compared to the *meso*-tetraaryl analogues.

Here, we report the conversion of *meso*-tetrahexyl-7,8-dihydroxychlorin into pyrrole-modified porphyrins via a range of oxidation and addition reactions. The products were characterized by UV–vis spectroscopy, NMR spectroscopy, and mass spectrometry. Comparisons with the corresponding tetraaryl-derived pyrrole-modified analogues are also presented. Collectively, these results delineate how alkyl substitution influences porphyrin core transformation pathways and reactivity.



REFERENCES

1. Brückner, C. The Breaking and Mending of *meso*-Tetraarylporphyrins: Transmuting the Pyrrolic Building Blocks. *Acc. Chem. Res.* **2016**, *49*, 1080−1092.
2. Luciano, M. P.; Atoyebi, A. O.; Tardie, W.; Zeller, M.; Brückner, C. Pyrrole-Modified Porphyrins Containing Eight-Membered Heterocycles Using a Reversal of the "Breaking and Mending" Strategy. *J. Org. Chem.* **2020**, *85*, 15273.
3. Wiehe, A.; Shaker, Y. M.; Brandt, J. C.; Mebs, S.; Senge, M. O. Lead Structures for Applications in Photodynamic Therapy. Part 1: Synthesis and Variation of *m*-THPC (Temoporfin) Related Amphiphilic A_2BC-Type Porphyrins. *Tetrahedron* **2005,** *61*, 5535−5564.
4. Aicher, D.; Damunupola, D.; Stark, C. B. W.; Wiehe, A.; Brückner, C. *meso*-Tetrahexyl-7,8-Dihydroxychlorin and Its Conversion to ß-Modified Derivatives. *Molecules* **2024**, *29*, 2144.

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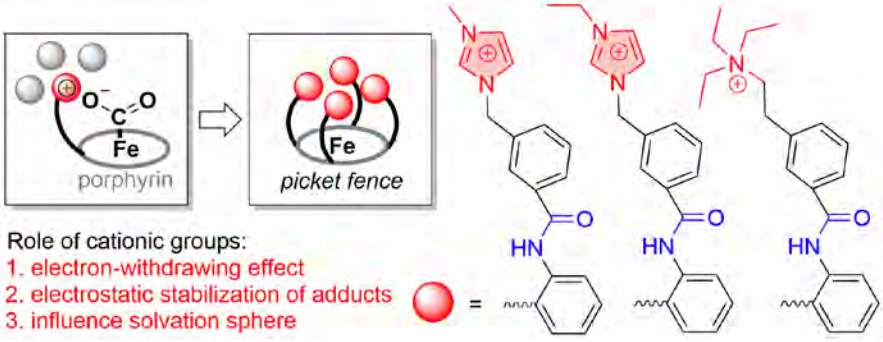
When Charge Matters: Electrostatic Second-Sphere Design Unlocks Enhanced Photocatalytic CO_2 Reduction

Albert Buenos[a], Asma Khadharoui[b], Ally Aukauloo[b], Zakaria Halime[b], Anja Krieger-Liszkay[a] ,Philipp Gotico[a]

[a] *Frédéric Joliot Institute for Life Sciences, French Atomic Energy and Alternative Energies Commission (CEA), Saclay 91400, France*
[b] *Institute of Molecular Chemistry and Materials of Orsay (ICMMO), Orsay 91190, France*

Breaking the linear scaling barrier in carbon dioxide reduction reaction (CO_2RR) remains a central challenge: boosting turnover frequency typically comes at the cost of higher overpotential. Nature, however, offers a blueprint. Enzymes such as carbon monoxide dehydrogenase seamlessly integrate multiple second coordination sphere interactions within a confined active site to orchestrate substrate binding, proton transfer, and charge stabilization with remarkable efficiency. Hydrogen-bond donors promote CO_2 capture and activation [1], while strategically positioned cationic residues stabilize anionic intermediates and reshape the local electric field [2-3].

Inspired by this strategy, we interrogate how electrostatic second-sphere effects can be deliberately tuned under photocatalytic conditions, where catalytic reactivity must align with the thermodynamics of the photoreductant. We report a multifunctional picket-fence iron porphyrin that combines a proximal amide with four cationic pendants, delivering a pronounced enhancement in CO production relative to the parent scaffold. Strikingly, subtle variation of the cationic substituent, from methyl-imidazolium to ethyl-imidazolium and ultimately to ethyl ammonium, leads to marked differences in CO2RR performance, revealing an unexpected sensitivity to second-sphere structure. Through a synergistic suite of *in situ* spectroscopy, laser flash photolysis, and spectroelectrochemistry, we uncover how fine-tuning electrostatics reprograms catalytic energetics under photocatalytic turnover.



REFERENCES

1. E. Pugliese et al. "Dissection of Light-Induced Charge Accumulation at a Highly Active Iron Porphyrin: Insights in the Photocatalytic CO_2 Reduction" *Angew Chem Int Ed.* **2022**, *61*, e202117530.
2. A. Khadhraoui et. al. "Through-Space Electrostatic Interactions Surpass Classical Through-Bond Electronic Effects in Enhancing CO_2 Reduction Performance of Iron Porphyrins" *ChemSusChem*. **2021**, *14*, 1308–1315.
3. M. R. Narouz et. al. "Multifunctional Charge and Hydrogen-Bond Effects of Second-Sphere Imidazolium Pendants Promote Capture and Electrochemical Reduction of CO_2 in Water Catalyzed by Iron Porphyrins" *Angew Chem Int Ed.* **2022**, *61*, e202207666.

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Novel A_3B-type phthalocyanine as building block for self-assembled nanoparticles with type I photodynamic and photothermal activity

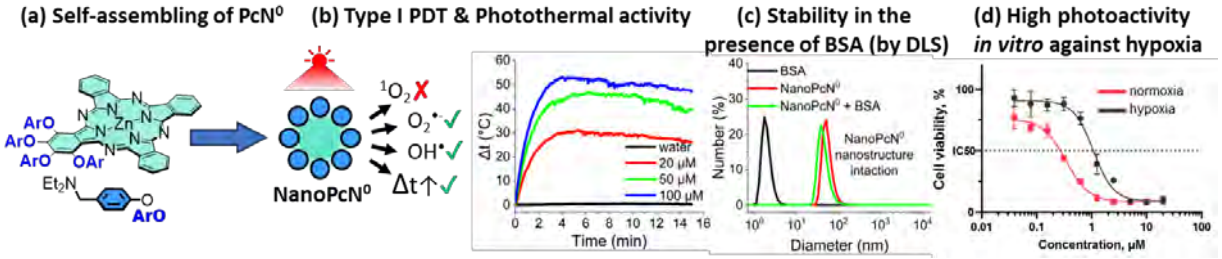
Dmitry A. Bunin[a], Tatiana V. Egorova[a,b], Polina P. Shram[a,b], Roman A. Akasov[c], Svetlana V. Monich[a,d], Maxim E. Stepanov[c], Maria P. Stepanova[a,e], Ekaterina K. Urodkova[a], Ivan N. Senchikhin[a], Alexander G. Martynov[a], Aslan Yu. Tsivadze[a,f] and Yulia G. Gorbunova[a,f]

[a]*Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, Moscow, Russia*
[b]*Department of Biochemistry, Petrovsky Medical University, Moscow, Russia*
[c]*Moscow Pedagogical State University (MPGU), Moscow, Russia*
[d]*Chemistry Department, Lomonosov Moscow State University, Moscow, Russia*
[e]*Faculty of Chemistry, National Research University Higher School of Economics, Moscow, Russia*
[f]*Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, Moscow, Russia*

POSTERS

One of the main advantages of photodynamic therapy (PDT) is its high spatial and temporal selectivity. The therapeutic effect of PDT is based on the generation of oxygen radicals (type I photoreactions) and singlet oxygen (type II photoreactions). The effectiveness of type I photoreactions is less dependent on oxygen content [1]. Therefore, photosensitizers that generate oxygen radicals may be useful for alleviating tumour hypoxia [2, 3].

Here, we obtained red-light-activated nanoparticles, NanoPcN^0, using nanoprecipitation of amphiphilic zinc(II) 1,2,3,4-tetrakis(4-(diethylaminomethyl)phenoxy)phthalocyaninate PcN^0 [4] (Fig. a). These nanoparticles generate $O_2^{\bullet-}$ [5] and OH$^\bullet$ (Fig. b) and demonstrate concentration-dependent photothermal conversion (Fig. b). NanoPcN^0 remains stable in the presence of bovine serum albumin (BSA, by DLS, Fig. c) and exhibit high photodynamic activity against MCF-7 tumour cells under both normoxic and hypoxic conditions (660 nm, 3.7 J/cm², Fig. d).



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REFERENCES

1. K.-Xu Teng et al., *Angew. Chem. Int. Ed.*, **2025**, 64, e202509416.
2. T. Xiong et al., *Small*, **2025**, 21, 2501911.
3. D. A. Bunin et al., *Biophys. Rev.*, **2023**, 15, 983–998.
4. D. A. Bunin et al., *J. Med. Chem.*, **2025**, 68, 658–673.
5. D. A. Bunin et al., *Opt. Mater.*, **2026**, 172, 117831.

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Engineering Non-Metalated Phtalocyanines on Au(111)

Lenka Černa,[a] Alba García-Frutos,[a] Ana Barragán,[a,b] Gouri Sahoo,[a] Sofia O. Perreiras,[a] Koen Lauwaet,[a] Óscar Jóver,[c] José I. Urgel,[a,b] Marco di Giovannantonio,[c] José I. Martínez,[d] Willi Auwärter,[e] José M. Gallego,[d] Ángela Sastre,[f] and David Écija[a,b]

[a] *Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nanoscience), 28049 Madrid, Spain*
[b] *Unidad de Nanomateriales Avanzados, Unidad Asociada al CSIC por el ICMM, 28049 Madrid, Spain*
[c] *CNR-Istituto Di Struttura della Materia (CNR-ISM), 00133 Roma, Italy*
[d] *Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC, 28049 Madrid, Spain*
[e] *Physik Department E20, Technische Universität München, 85748 Garching, Germany*
[f] *Área de Química Orgánica, Instituto De Bioingeniería, Universidad Miguel Hernández, Elche, Spain*

Silicon phthalocyanine (Cl_2SiPc) is a promising molecular platform for surface-supported catalysis due to the hexacoordinated silicon center with tunable axial ligands. In its dichlorinated form, however, the axial chlorine atoms block access to the Si center, limiting its chemical reactivity. It is therefore desirable to perform catalysis directly with the SiPc species. Here, we demonstrate the controlled on-surface dechlorination of Cl_2SiPc on Au(111), enabling the exposure of a coordinatively accessible Si center and thereby activating the molecule for potential catalytic applications. [1-2] Cl_2SiPc precursors were deposited under ultra-high vacuum conditions and characterized by scanning tunneling microscopy (STM), non-contact atomic force microscopy (nc-AFM), and X-ray photoelectron spectroscopy (XPS). Upon adsorption at room temperature, the surface predominantly populated by mono-chlorinated Cl–SiPc species, with a minor fraction of fully dechlorinated SiPc. Subsequent thermal annealing induces complete cleavage of the remaining Si–Cl bonds, yielding SiPc molecules with an exposed silicon center. The ability to controllably remove axial chlorine ligands under surface-confined conditions provides a direct route to generate coordinatively unsaturated Si sites in individual phthalocyanines. Such exposed Si centers are predicted to act as single-site catalytic centers capable of promoting spontaneous N_2O dissociation. [3]

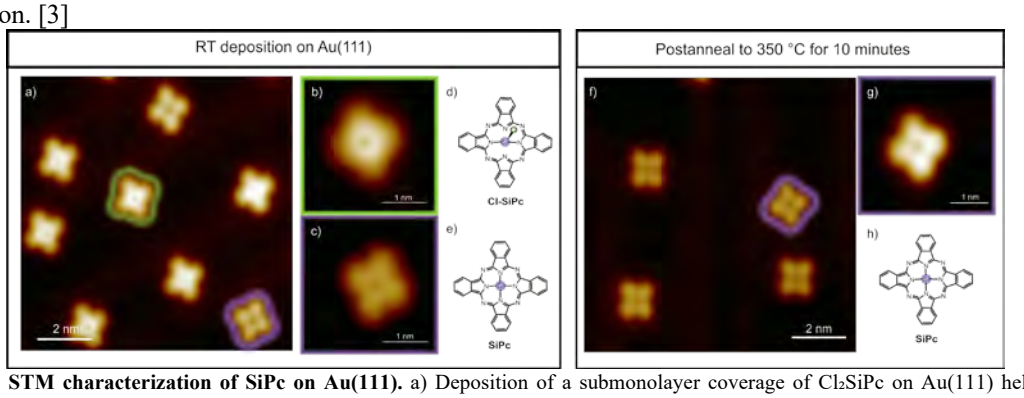


Figure 1. STM characterization of SiPc on Au(111). a) Deposition of a submonolayer coverage of Cl_2SiPc on Au(111) held at room temperature, illustrating the predominant Cl–SiPc species (highlighted by green line) coexisting with a minor fraction of Cl-free SiPc species (highlighted by violet line). V = 600 mV, I = 10 pA. b) High resolution STM image of a Cl–SiPc species. V = 500 mV, I = 10 pA. c) High resolution STM image of a SiPc species. V = 500 mV, I = 10 pA. d,e) Chemical models of Cl–SiPc and SiPc species, respectively. f) Long range STM image after annealing a) at 350 °C for 10 minutes. V = 100 mV, I = 10 pA. g) High resolution STM image of a SiPc species in agreement to c). V = 500 mV, I = 50 pA. h) Chemical model of SiPc.

REFERENCES

1. Baklanov, Aleksandr et al., *JACS*, 142.4 (2020): 1871-1881.
2. Mitra, Koushambi, and Matthew CT Hartman, *Organic & Biomolecular Chemistry* 19.6 (2021): 1168-1190.
3. Khan, Adnan Ali et al., *Physical Chemistry Chemical Physics* 26.24 (2024): 17110-17117.

POSTERS

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Chitosan-based sponge loaded with zinc phthalocyanine as a multifunctional wound dressing material

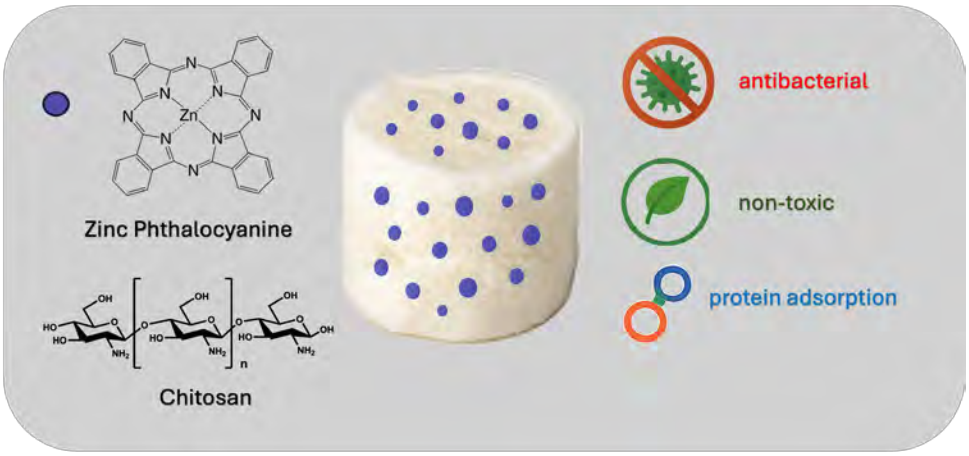
Dorota Chelminiak-Dudkiewicz[a], **Aleksander Smolarkiewicz-Wyczachowski**[a], **Kinga Mylkie**[a], **Marta Ziegler-Borowska**[a]

[a] *Department of Biomedical Chemistry and Polymer Science, Medicinal Chemistry Research Group, Faculty of Chemistry, Nicolaus Copernicus University in Torun, Gagarina 7, 87-100, Torun, Poland*

The skin serves as a crucial protective barrier, and its damage significantly increases the risk of infection and delayed healing. Therefore, the development of advanced wound-dressing materials that combine biocompatibility, mechanical stability, and antimicrobial activity remains a significant challenge. In this study, a chitosan-based sponge loaded with zinc phthalocyanine was developed as a multifunctional wound dressing.

Chitosan was selected for its excellent biocompatibility, biodegradability, antioxidant properties, and its ability to support tissue regeneration. Zinc phthalocyanine was introduced to enhance the system's antibacterial activity, particularly against drug-resistant microorganisms. The obtained sponge was characterized for its physicochemical properties and biological performance. Additionally, interactions with human serum albumin were investigated to evaluate the material's behavior in a biological environment.

The results indicate that the developed chitosan/zinc phthalocyanine sponge exhibits properties desirable for wound-dressing applications, including favorable material–protein interactions and functional characteristics that support its biomedical use. This study highlights the potential of chitosan-based composite sponges as advanced wound dressing materials.



REFERENCES

1. Y. Feng, X. Li, Q. Zhang, S. Yan, Y. Guo, M. Li, R. You, Mechanically robust and flexible silk protein/polysaccharide composite sponges for wound dressing, Carbohydrate Polymers, 216 (2019) 17-24.
2. M. Ji, J. Li, Y. Wang, F. Li, J. Man, J. Li, C. Zhang, S. Peng, S. Wang, Advances in chitosan-based wound dressings: Modifications, fabrications, applications and prospects, Carbohydrate Polymers, 297 (2022) 120058.

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Cyclodextrin-Conjugated Phthalocyanines as Tumor-Targeting and Renal-Clearable Photosensitizers for Photodynamic Therapy

Zhaolin Chen[a], Yunong Xie[b], Minghe Zhang[b], Man Tong[b], Evelyn Y. Xue*[a,c], and Dennis K. P. Ng*[a]

[a] *Department of Chemistry, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China*
[b] *School of Biomedical Sciences, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China*
[c] *Department of Biomedical Engineering, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China*

Photodynamic therapy (PDT) has emerged as a highly effective and non-invasive approach for cancer treatment [1]. However, a significant clinical limitation arises from the persistent photosensitivity induced by the residual photosensitizer. Consequently, it is crucial to develop strategies that can effectively eliminate this photoacive agnet after the treatment [2]. To this end, we utilized β-cyclodextrin moieties to promote the renal clearance of a zinc(II) phthalocyanine (ZnPc) core used as the photosensitizer. Through systematic screening the in vivo renal-clearable property of a series of ZnPcs substituted with 1, 2, or 4 β-cyclodextrin unit(s), we found that the disubstituted analogue (Pc-2CD) exhibited the best performance, which was therefore selected for the subsequent studies. To achieve targeted delivery, adamantane conjugated with an epidermal growth factor receptor (EGFR)-targeting peptide was used to selectively label EGFR-overexpressed cancer cells and tumors in nude mice for complexation with Pc-2CD through host-guest interactions. It resulted in enhanced localization of the photosensitizer at the target site, leading to high PDT efficacy upon light irradiation. Interestingly, the residual photosensitizer was efficiently excreted via the kidneys, and no significant skin phototoxicity was observed upon light irradiation. The overall results show that this supramolecular photosensitizing system can facilitate targeted PDT without causing post-treatment photosensitivity, rendering this approach highly promising for clinical translation.

This work was supported by a General Rsearch Fund from the Research Grants Council of the Hong Kong Special Administrative Region, China (ref. no. 14307924).

REFERENCES

1. Dolmans, D. E. J. G. J.; Fukumura, D.; Jain, R. K. Photodynamic therapy for cancer. *Nat. Rev. Cancer* **2003**, *3*, 380−387.
2. Xue, E. Y.; Yang, C.; Zhou, Y.; Ng, D. K. P. A bioorthogonal antidote against the photosensitivity after photodynamic therapy. *Adv. Sci.* **2024**, *11*, 2306207 and the references cited therein.

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EGFR-Targeted Antibody–Polymer–Photosensitizer Induces ROS-Mediated Immunogenic Cell Death and Suppresses KRAS-Driven Signaling in Colorectal Cancer

Hani Choi[a,b], Kun Na[a,b,*]

[a] *Department of BioMedical-Chemical Engineering, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Bucheon-si, Gyeonggi-do 14662, Republic of Korea*
[b] *Department of Biotechnology, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Bucheon-si, Gyeonggi-do 14662, Republic of Korea*

** Corresponding author: Department of BioMedical-Chemical Engineering, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Bucheon-si, Gyeonggi-do 14662, Republic of Korea*

Conventional antibody–drug conjugates (ADCs) face therapeutic limitations in KRAS-mutated colorectal cancer (CRC). In response, we developed EPP (EGFR Antibody–Polymer–Photosensitizer), a targeted photoactivatable platform combining EGFR-directed delivery with photodynamic therapy (PDT). EPP is composed of an EGFR-targeting antibody conjugated with a biocompatible polymer- photosensitizer conjugate. This structural design facilitates tumor-selective accumulation and enables light-triggered therapeutic activation. Following laser irradiation, EPP produces reactive oxygen species (ROS), triggers immunogenic cell death, and inhibits ERK and AKT signaling pathways. EPP exhibited potent antitumor efficacy both *in vitro* and *in vivo*, achieving over 90% cytotoxicity *in vitro* and reducing tumor growth by 90% in KRAS-mutated CRC models. In addition, EPP promoted systemic antitumor immunity by increasing dendritic cell and $CD8^+$ T cell populations and reducing regulatory T cells. Collectively, these results demonstrate that EPP exerts dual antitumor functions through direct targeting of tumor cells and modulation of the immune microenvironment. This dual mechanism presents a promising therapeutic strategy to overcome KRAS-associated resistance in colorectal cancer.

REFERENCES

1. J. Kim, W. Park, D. Kim, E. S. Lee, D. H. Lee, S. Jeong, J. M. Park, K. Na, *Adv. Funct. Mater. 2019, 29, 1900084.*
2. A. Hak, M. S. Ali, S. A. Sankaranarayanan, V. R. Shinde, A. K. Rengan, *ACS Appl. Bio Mater. 2023, 6, 349.*
3. J. W. Buecheler, M. Winzer, J. Tonillo, C. Weber, H. Gieseler, *Mol. Pharmaceutics 2018, 15, 2656.*

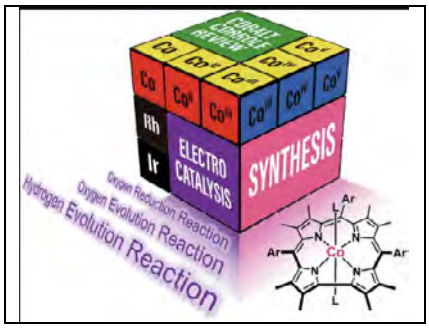
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Cobalt Corroles and their Level of Hydrogen Evolution Activity

David G. Churchill [a,b], **Jyoti** [c], **Ritika Kubba** [c], **Sachin Kumar** [d], **Natalia Fridman** [d], **Sudhir G. Warkar** [c] **Anil Kumar** [d]

[a]*KAIST, Department of Chemistry, Molecular Logic Gate Laboratory, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Republic of Korea.* [b]*Therapeutic Bioengineering Section, KAIST Institute for Health Science and Technology (KIHST), Daejeon, Republic of Korea.* [c]*Department of Applied Chemistry, Delhi Technological University, Delhi, 110042, India.* [d]*Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Haifa, Israel.*



In this work, electrochemical studies of a series A_2B Cobalt corroles were carried out.[1] Differences in the impact of the corrole's electron withdrawing/donating groups (EWG and EDGs) present on the phenyl groups at meso-positions was evaluated in this published study.[2] The complexes were examined for hydrogen evolution reaction (HER) activity. The complexes do not show activity toward the HER; rather they supply ligands for the process. The meso-corrole substituents have significant effect on the overall activity of Co macrocycles. Substitution with electron withdrawing or donating groups has an effect on the corrole's overall oxidation or reduction potential which was assessed through the use of cyclic voltametric (CV) experiments. Additionally, DFT methods were used to assess the influence of meso-substituents and to structurally optimize the geometries of the complexes to help our understanding of the sometimes-subtle structural characteristics found in the macromolecular systems. The compound involved is a novel penta-coordinated triphenylphosphine ligated corrole *i.e.*, [10-(2,6-difluorophenyl)-5,15-bis(4-nitrophenyl)corrolato]cobalt(III)·pyridine was also synthesised and characterized using spectroscopic techniques and structurally studied via X-ray diffraction.

REFERENCES

1. Jyoti, An, J., Kim, D., Churchill, D. G., Kumar, A. "Cobalt corroles: Synthesis and applications." Coordination Chemistry Reviews **2024**, 511, 215869.
2. Jyoti, Kubba, R., Kumar, S., Fridman, N., Warkar, S. G., Churchill, D. G., Kumar A. « Hydrogen evolution activity of cobalt corroles. » Inorganica Chimica Acta **2024**, 562, 121878.

POSTERS

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Covalently linked porphyrin-carbon dot hybrids for efficient visible light hydrogen production

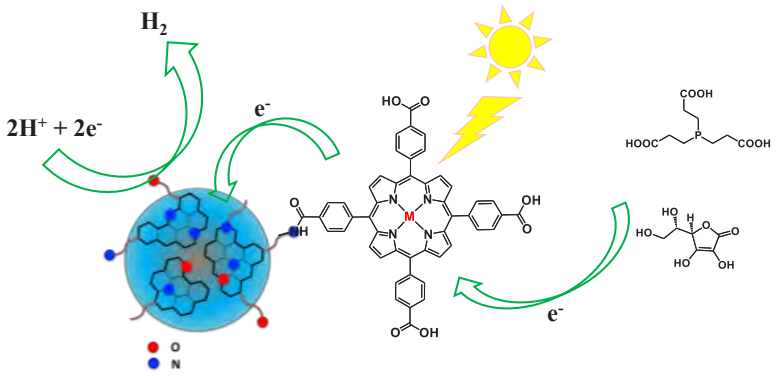
Athanassios G. Coutsolelos[a,b], Katerina Achilleos[a], Anna Katsari[a], Emmanuel Nikoloudakis[a,b], Georgios Charalambidis[c], Kalliopi Ladomenou[d]

[a]*Laboratory of Bioinorganic Chemistry, Chemistry Department, University of Crete, 70013 Heraklion, Crete, Greece.*
[b]*Foundation for Research and Technology (FORTH), Institute of Electronic Structure and Laser (IESL), 70013, Heraklion, Greece.*
[c]*Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., 11635, Athens, Greece.*
[d]*Hephaestus Laboratory, School of Chemistry, Faculty of Sciences, Democritus University of Thrace, Kavala, Greece.*

The development of sustainable photocatalytic systems for hydrogen production is crucial for solar-to-fuel energy conversion. In this study, hybrid nanomaterials consisting of porphyrin derivatives covalently linked to nitrogen-doped carbon dots (NCDots) were synthesized and investigated as water-soluble photocatalysts for visible-light-driven hydrogen evolution. The hybrids were prepared via amide coupling between tetra-carboxyphenyl porphyrins (TCPP, ZnTCPP) and surface amino groups of NCDots. Spectroscopic and structural characterization (UV–Vis, fluorescence, FT-IR, NMR, XPS, and SEM) confirmed successful functionalization and strong electronic interaction between the components.

Photocatalytic experiments under visible light revealed that the ZnTCPP–NCDots hybrid exhibits significant hydrogen production in aqueous solution using a TCEP/ascorbic acid sacrificial donor system, reaching up to 9 mmol g^{-1} after prolonged irradiation. Control experiments demonstrated that covalent coupling is essential for efficient photoinduced charge transfer.

These results highlight porphyrin–carbon dot hybrids as promising noble-metal-free photocatalysts for solar hydrogen generation.



REFERENCES

1. K. Achilleos, A. Katsari, E. Nikoloudakis, F. Chatzipetri, D. Tsikritzis, K. Ladomenou, G. Charalambidis, E. Stratakis and A. G. Coutsolelos, *Dalton Trans.,* 2025, 54, 328 DOI: 10.1039/d4dt02101k.
2. A. Charisiadis, V. Nikolaou, E. Nikoloudakis, K. Ladomenou, G. Charalambidis and A. G. Coutsolelos, *Chem. Commun*., 2025, 61, 4630-4646 DOI : 10.1039/D4CC06655C.

POSTERS

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Synthesis and Structural Evolution of Lanthanide-Porphyrin MOFs

Russell D. Cox[a], **Ian Russell**[a], **Amy E. Hixon**[a]

[a]*Department of Civil & Environmental Engineering & Earth Sciences, University of Notre Dame, Notre Dame, IN, 46556, USA.*

Metal-organic frameworks (MOFs) are a class of crystalline porous materials that have highly tunable structures and functionalities [1]. Lanthanide-porphyrin MOFs possess immense potential for advanced sensing and photocatalysis due to their unique electronic [2] and magnetic properties [3], yet they remain underrepresented in structural databases compared to transition-metal frameworks. Due to the challenges of growing large single crystals under application-specific conditions, researchers frequently rely on matching microcrystalline powder patterns to known structures, a "fingerprinting" method that often obscures critical structural nuances. Through a non-traditional heteronuclear seeding approach, we report the successful synthesis and structural characterization of a series of lanthanide metal-organic frameworks from La to Lu that incorporate tetrakis(4-carboxyphenyl)porphyrin (TCPP) as the organic linker. X-ray diffraction, vibrational spectroscopy, electron microscopy, and nitrogen adsorption-desorption isotherms were used to define and describe a structural evolution that results from the lanthanide contraction [4]. The lanthanide contraction influences coordination number of the metal center in the chains that form the secondary building unit (SBU), which pushes the resulting framework topologies into two categories: (i) an S-topology in the early-mid lanthanides corresponding to a low symmetry (P-1) space group and (ii) a Z-topology in the late lanthanides corresponding to a higher symmetry (*Pccn*/*Pbnb*) space group. This structural shift dictates the porphyrin arrangement by governing their tilt angles relative to the SBU, the extent of face-to-face interactions, and, in the case of the later lanthanides, the formation of isolated pore pockets. These results highlight that, while the lanthanides have the same oxidation state and similar chemical properties, the small deviances generated by the lanthanide contraction influence coordination geometry to such an extent that they can govern the macroscopic architecture and periodicity in MOFs.

REFERENCES

1. Safaei, M.; Foroughi, M. M.; Ebrahimpoor, N.; Jahani, S.; Omidi, A.; Khatami, M. A Review on Metal-Organic Frameworks: Synthesis and Applications. TrAC Trends Anal. Chem. **2019**, 118, 401–425. https://doi.org/10.1016/j.trac.2019.06.007.
2. Li, D.; Yadav, A.; Zhou, H.; Roy, K.; Thanasekaran, P.; Lee, C. Advances and Applications of Metal-Organic Frameworks (MOFs) in Emerging Technologies: A Comprehensive Review. Glob. Chall. **2024**, 8 (2), 2300244. https://doi.org/10.1002/gch2.202300244.
3. Furukawa, H.; Cordova, K. E.; O'Keeffe, M.; Yaghi, O. M. The Chemistry and Applications of Metal-Organic Frameworks. Science **2013**, 341 (6149), 1230444. https://doi.org/10.1126/science.1230444.
4. Shannon, R. D. Revised Effective Ionic Radii and Systematic Studies of Interatomic Distances in Halides and Chalcogenides. Acta Crystallogr. Sect. A **1976**, 32 (5), 751–767. https://doi.org/10.1107/S0567739476001551.

POSTERS

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Porphyrin-based Plutonium Metal–Organic Frameworks: A Versatile Platform for Investigating Elusive Actinide Cluster Chemistry

Russell D. Cox[a], **Amy E. Hixon**[a]

[a]*Department of Civil & Environmental Engineering & Earth Sciences, University of Notre Dame, Notre Dame, IN, 46556, USA.*

Plutonium coordination chemistry has evolved rapidly over the last decade, transitioning from fundamental studies of 1D and 2D coordination polymers[1] to the realization of complex 3D metal-organic frameworks (MOFs)[2]. Following the landmark 2020 synthesis of Pu-UiO-66 [3], interest has intensified in leveraging these porous scaffolds to stabilize elusive coordination environments and high-coordination nodes that are typically inaccessible via traditional high-temperature solid-state methods. Because MOFs offer a modular platform for nanoscale control, they are uniquely suited for investigating the distinct relativistic effects and *f*-orbital participation in bonding that characterize the tetravalent actinides. In this study, we report the solvothermal synthesis of a plutonium-based MOF incorporating the tetrakis(4-carboxyphenyl)porphyrin (TCPP) organic linker. Using a modulated solvothermal approach with trifluoroacetic acid, we successfully obtained a microcrystalline material that preliminary characterization via powder X-ray diffraction (PXRD) suggests is isostructural with the PCN-222 framework. While initial crystal dimensions were restricted to the microscale (10–50 μm), we observed a significant morphological and structural evolution over 14-months. This aging process, likely driven by radiolytically-induced Ostwald ripening, resulted in the growth of significantly larger crystals reaching 250 μm in length. However, analysis using single-crystal X-ray diffraction (SCXRD), PXRD, and Raman spectroscopy suggests that long-term exposure to ionizing radiation may have triggered a phase transition from the original porous framework into a high-symmetry plutonium compound, tentatively assigned as a plutonium oxyhydroxide. Central to this research is the exploitation of the porphyrin linker's inherent photophysical properties as a tool for structural investigation. Porphyrins exhibit a known susceptibility to oxidative ring breakdown under specific light excitation. We hypothesize that "surgical" photocleavage can be used to systematically degrade the organic framework to isolate and study the stabilized plutonium clusters without the structural damage caused by traditional harsh chemical reagents. This work, supported by a comprehensive synthetic roadmap developed across the lanthanide series (La–Yb), establishes a new transuranic architecture and provides a vital methodology for evaluating the impact of long-term self-radiolysis on the stability and transformation of actinide-based porous materials.

REFERENCES

1. Charushnikova, I. A.; Fedoseev, A. M.; Bessonov, A. A. Crystal Structure of An(VI) Complexes with Succinate Anions, $[PuO_2(C_4H_4O_4)(H_2O)]$ and $Cs_2[(AnO_2)_2(C_4H_4O_4)_3]\cdot H_2O$ (An = U, Np, Pu). Radiochemistry **2019**, 61 (2), 137–145. https://doi.org/10.1134/S1066362219020024.
2. Hastings, A. M.; Ray, D.; Jeong, W.; Gagliardi, L.; Farha, O. K.; Hixon, A. E. Advancement of Actinide Metal–Organic Framework Chemistry via Synthesis of Pu-UiO-66. J. Am. Chem. Soc. **2020**, 142 (20), 9363–9371. https://doi.org/10.1021/jacs.0c01895.
3. Lv, K.; Urbank, C.; Patzschke, M.; März, J.; Kaden, P.; Weiss, S.; Schmidt, M. MOFs with 12-Coordinate 5f-Block Metal Centers. J. Am. Chem. Soc. **2022**, 144 (7), 2879–2884. https://doi.org/10.1021/jacs.1c13127.

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Long-lived Excited Charge Separation in Silicon(IV) Phthalocyanine with Axially Bound C_{60} *via* Azobenzene Spacers

Andrew W. Dawson[a], Victor Sobrino-Bastán[b], Luis Martín-Gomis[b], Ángela Sastre-Santos*[,b], and Francis D'Sozua*[,a]

[a]*Department of Chemistry, University of North Texas, 1155 Union Circle, #305070, Denton, TX 76203-5017, USA*
[b]*Área de Química Orgánica, Instituto de Bioingeniería, Universidad Miguel Hernández, Avda. de la Universidad s/n, 03203 Elche, Spain*

A very important characteristic of modern artificial photosynthetic systems used in energy-conversion applications is accelerated charge separation and long-lived charge-separated states. [1] Phthalocyanines have been used extensively as strong electron-donating groups in donor-acceptor systems; however, p-block element-hosting phthalocyanines have yet to be fully investigated. [2-3] A novel silicon(IV) phthalocyanine, SiPc-derived donor-acceptor, has been synthesized, with two C_{60} electron-accepting groups attached to the axial positions of the SiPc *via* azobenzene spacers. The *trans*-to-*cis* isomerization, which adjusts the donor-acceptor distance, was achievable upon photoirradiation; however, this process was accompanied by considerable photodecomposition of the triad. Strong fluorescence quenching was observed in the *trans*-C_{60}-azo-SiPc-azo-C_{60} compared to the SiPc control, suggesting the occurrence of excited-state nonradiative processes upon photoexcitation. Electrochemical and spectroelectrochemical studies were performed to determine the redox potentials and to help identify the electron-transfer products, $SiPc^{\bullet+}$ and $C_{60}^{\bullet-}$. The subsequently constructed energy diagram indicated that electron transfer occurs from ^{1}SiPc* to C_{60} in the triad, then relaxes to the ^{3}SiPc* state before returning to the ground state. This electron-transfer mechanism was also supported by the DFT and TD-DFT calculations, with analysis using MultiWFN. Femtosecond transient absorption studies verified electron transfer from ^{1}SiPc* to C_{60} in the triad, with the products, $SiPc^{\bullet+}$ and $C_{60}^{\bullet-}$, being spectrally identifiable. In the donor-acceptor triad, the ^{1}SiPc* had lifetimes of 86.81 and 65.91 ps in toluene and benzonitrile, respectively, which were significantly shorter than those of the SiPc-control. The final lifetimes of the radical ion pair $SiPc^{\bullet+}$-$C_{60}^{\bullet-}$ in the triad, based on nanosecond transient absorption studies, were determined to be 589.5 and 561.4 ns for $SiPc^{\bullet+}$ and $C_{60}^{\bullet-}$ signals, respectively, in toluene, and 433.8 and 488.0 ns for $SiPc^{\bullet+}$ and $C_{60}^{\bullet-}$ signals, respectively, in benzonitrile. The lifetime of the ^{3}SiPc* formed during charge recombination was found to be 6.04 and 5.95 μs in toluene and benzonitrile, respectively, close to that of the SiPc-control in each solvent. The long-lived charge-separated states enable this triad to serve as a platform for further photocatalytic and optoelectronic applications.

REFERENCES

1. Dawson AW, Sobrino-Bastán V, Martín-Gomis L, Sastre-Santos Á and D'Souza F. *J. Porphyrins Phthalocyanines* 2025; **29**: 1093-1106.
2. Martín-Gomis L, Seetharaman S, Herrero D, Karr PA, Fernández-Lázaro F, D'Souza F and Sastre-Santos Á. *ChemPhysChem* 2020; **21**: 2254-2262.
3. Lee W, Zhan X, Palma J, Vestfrid J, Gross Z and G. Churchill D. *Chem. Commun.* 2021; **57**: 4605-4641.

POSTERS

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Development of new building blocks based on phosphonic acid corroles for the preparation of porous materials for gas detection

Gaëlle Divoux, Margerie Loze, Laurie André, Stéphane Brandès, Claude P. Gros, Nicolas Desbois

ICMUB, UMR CNRS 6302, Université Bourgogne Europe, 9 avenue Alain Savary, 21000 Dijon, France

Monitoring air quality has become an important challenge in order to prevent damage to human health and the environment. It is therefore essential to develop suitable and sensitive sensors to detect dangerous gases, such as CO or NH_3, at very low concentrations. For several years, our laboratory has been interested in the development of cobalt corroles that can selectively and reversibly coordinate CO or NH_3 [1]. To improve gas access, porous materials, such as Metal Organic Frameworks (MOFs) have attracted our attention due to their high porosity and high tunability. Our idea is to graft cobalt corroles onto MOFs and deposit these materials on SAW (Surface Acoustic Wave) sensors which can be used to detect low concentrations of gas. Until now we have only used corroles functionalized with a carboxylic acid to construct materials [2]. In this work, we propose to develop a new family of corroles with a phosphonic acid function. We will present the synthesis of these new precursors and also give preliminary results on the grafting of these compounds onto a porphyrin-based MOFs (PCN-222). These new materials have been characterized by mass spectrometry, multinuclear NMR spectroscopy and UV-Visible but also by BET, XRD, gas adsorption (CO, N_2, O_2 and CO_2) [3].

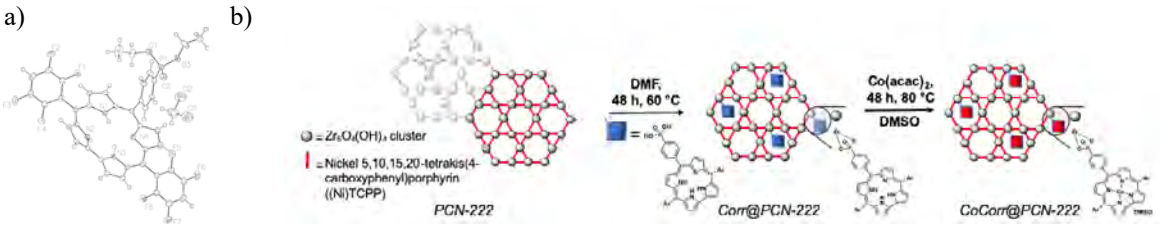


Figure 1. X-ray structure of synthesized phosphonate corrole. b) Grafting of phosphonic acid corrole into the porphyrin-based metal organic framework

This work was supported by the CNRS (UMR UB-CNRS 6302) and the Université Bourgogne Europe (UBE). The French Research Agency (ANR) is acknowledged for financial support (ANR-22-CE42-0016-02).

REFERENCES

1. (a) Brandès, S; Quesneau, V.; Fonquernie, O.; Desbois, N.; Blondeau-Patissier, V.; Gros C. P. *Dalton Trans.*, **2019**, 48 (31), 11651-11662; (b) Vanotti, M.; Poisson, S.; Soumanna, V.; Quesneau, V.; Brandès, S.; Desbois, N.; Yang, J.; André, L.; Gros, C. P.; Blondeau-Patissier, V. *Sens. Actuator B-Chem*. **2021**, 332, 129507; (c) André, L.; Desbois, N.; Gros, C. P.; Brandès S. *Dalton Trans*., **2020**, 49 (43), 15161-15170.
2. Loze, M.; Brandès, S.; Fleurat-Lessard, P.; Desbois, N.; Blondeau-Patissier, V.; Gros, C. P.; André, L. *Chem. Eur. J.*, **2024**, *30*, e202402148
3. Divoux, G.; Loze, M.; Rousselin, Y.; Brandès, S.; Gros, C. P.; Desbois, N.; André, L. *Dalton Trans*. **2025**, 54, 1784-1790.

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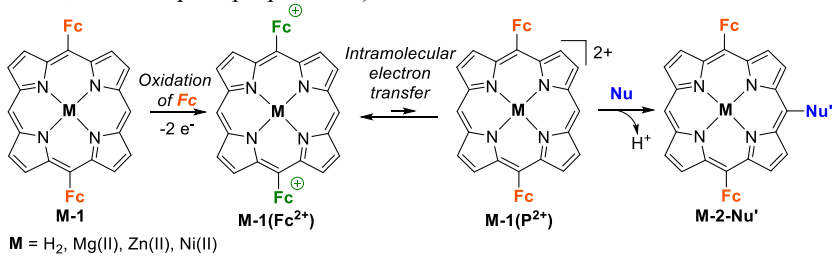


Intramolecular Electron Transfer Between Electrogenerated Ferrocenium and Porphyrin Redox Units: Application to *meso*-Functionalization of 5,15-bis-FerrocenylPorphyrin

Nesrine Amiri[a], Asmae Bousfiha[a], Fatima Akhssas[a], Abdou Khadre Djily Dimé[a], Hélène Cattey[a], Julien Roger[a] and Charles H. Devillers[a]

[a] *Université Bourgogne Europe, CNRS, Institut de Chimie Moléculaire de l'Université de Bourgogne (ICMUB, UMR CNRS 6302), 9 avenue Alain Savary, 21078 Dijon Cedex, France*

Porphyrins have been widely studied for over a century due to their versatile physico-chemical properties and ease of functionalization. Within this family, ferrocenyl-substituted porphyrins are of particular interest because electronic communication between the ferrocene unit and the porphyrin ring strongly depends on the position and nature of the linkage. These hybrid systems have found applications ranging from molecular sensing to information storage, catalysis, and antimicrobial materials. However, only a few 5- or 5,15-ferrocenylporphyrins bearing free meso positions exist, and meso-functionalization of ferrocenyl-porphyrins has not been reported.[1,2] Since more than a decade, our team is interested in electrochemically-driven porphyrin modification through intra- or intermolecular nucleophilic attack on porphyrin cation radicals.[3] We questioned ourself whether a bis-ferrocenium porphyrin, generated by removing two electrons from ferrocenyl groups, could undergo nucleophilic attack at remaining meso positions. This process would represent an unusual intramolecular electron-transfer-driven reaction between two electroactive fragments. Previous studies on related systems illustrate that such pathways, though seemingly unfavorable, can occur.[4] The present work thus reports the synthesis, characterization, and nucleophilic reactivity of several 5,15-bis-ferrocenylporphyrins (H_2, Mg(II), Zn(II), Ni(II), Scheme 1, *manuscript in preparation*).



Scheme 1. Anodic nucleophilic substitution of **M-1** by oxidation of the ferrocenyl (Fc) moieties.

REFERENCES

1. Suijkerbuijk, B. M. J. M.; Klein Gebbink, R. J. M. Merging Porphyrins with Organometallics: Synthesis and Applications. *Angew. Chem. Int. Ed.* **2008**, *47* (39), 7396–7421.
2. Bucher, C.; Devillers, C. H.; Moutet, J.-C.; Royal, G.; Saint-Aman, E. Ferrocene-Appended Porphyrins: Syntheses and Properties. *Coord. Chem. Rev.* **2009**, *253* (1–2), 21.
3. Bousfiha, A.; Amiri, N.; Akhssas, F.; Berthelot, M.; Echaubard, J.; Pirrotta, M.; Cattey, H.; Fleurat-Lessard, P.; Roger, J.; Devillers, C. H. Synthesis of Meso,β-Fused Thiazinamine-Porphyrins via Oxidative C–N Fusion of Pyrimidinyl-Substituted Porphyrins. *Org. Lett.* **2023**, *25* (44), 7979–7983.
4. Duan, S.; Moeller, K. D. Anodic Cyclization Reactions: Capitalizing on an Intramolecular Electron Transfer to Trigger the Synthesis of a Key Tetrahydropyran Building Block. *J. Am. Chem. Soc.* **2002**, *124* (32), 9368–9369.

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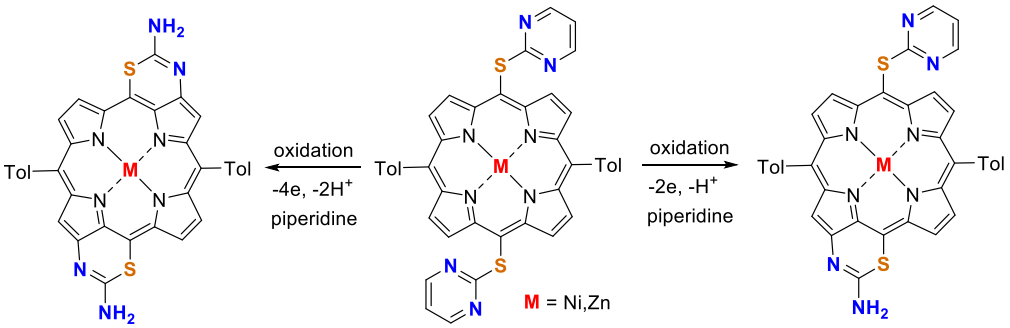


Synthesis of *meso*,β-fused Thiazinamine-Porphyrins via Oxidative C-N Fusion of Pyrimidinyl-substituted Porphyrins

Nesrine Amiri[a], Asmae Bousfiha[a], Fatima Akhssas[a], Mathieu Berthelot[a], Hélène Cattey[a], Julien Roger[a], Charles H. Devillers[a]

[a] *Université Bourgogne Europe, CNRS, Institut de Chimie Moléculaire de l'Université de Bourgogne (ICMUB, UMR CNRS 6302), 9 avenue Alain Savary, 21078 Dijon Cedex, France*

π-Extension of aromatic molecules via intramolecular C-C or C-N coupling(s) has long been of interest to numerous research teams [1, 2]. The C-C or C-N fused compounds demonstrate an important change in their electronic properties, such as bathochromic shift of their absorption/emission spectrum, two-photon cross-section increase, and HOMO-LUMO gap decrease. They found applications in photovoltaic cells, molecular electronics, photodynamic therapy, non-linear optical materials, and near-IR electroluminescence displays. In this work, 5,15-bis(pyrimidin-2-ylthio)porphyrins have been synthesized. Their electrochemical oxidation leads to the formation of the mono- and bis-C-N-fused thiopyrimidinium intermediates depending on the applied charge and potential. These latter undergo nucleophilic attack by water during work-up, which drives the ring-opening of the pyrimidinium moiety. When piperidine is added before or after work-up, the neutral fused porphyrinthiazin-2-amines are generated, and they exhibit a significant bathochromic shift of their Soret bands [3].



REFERENCES

1. Davis, N. K. S.; Thompson, A. L.; Anderson, H. L. A Porphyrin Fused to Four Anthracenes. *J. Am. Chem. Soc.* **2011**, *133*, 30–31.
2. Chen, Q.; Brambilla, L.; Daukiya, L.; Mali, K. S.; De Feyter, S.; Tommasini, M.; Müllen, K.; Narita, A. Synthesis of Triply Fused Porphyrin-Nanographene Conjugates. *Angew. Chem. Int. Ed.* **2018**, *57* (35), 11233–11237.
3. Bousfiha, A.; Amiri, N.; Akhssas, F.; Berthelot, M.; Echaubard, J.; Pirrotta, M.; Cattey, H.; Fleurat-Lessard, P.; Roger, J.; Devillers, C. H. Synthesis of Meso,β-Fused Thiazinamine-Porphyrins via Oxidative C–N Fusion of Pyrimidinyl-Substituted Porphyrins. *Org. Lett.* **2023**, *25* (44), 7979–7983.

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Electrochemical Conversion of Nitrate and Carbon Dioxide to Value-Added Chemicals Using Bifunctional Electrocatalyst Cobalt Tritolycarboxyl Porphyrin

Kamal Dhakal[a], Alankar Kafle[a], Diliraj Subedi[b], Mohammad K. Altafi[a], Alireza Hajiseyedjavadi[a], Swatej Sabbarwal[a], Thomas R. Cundari*[a] and Francis D'Souza*[a]

[a]*Department of Chemistry, University of North Texas at Denton, 1155 Union Circle, 305070, Denton, TX 76203-5017 (USA)*
[b]*Department of Natural Sciences, Hesston College, 301 South Main Street, Hesston, KS,67062, USA*

The electrochemical pathways for the nitrate reduction reaction (NO_3RR) and the carbon dioxide reduction reaction (CO_2RR) can serve as effective tools for remedying environmental pollutants, thereby supporting a circular economy. These electrochemical conversion processes depend strongly on the activity of the electrode materials. Therefore, the development of highly efficient and active electrocatalysts in an eco-friendly and cost-effective manner is crucial. This study examines the potential efficacy of cobalt porphyrins in combination with conductive carbon supports and peripheral functional-group modifications for the selective synthesis of ammonia and acetic acid/formic acid via electrochemical reduction of nitrate and carbon dioxide, respectively. The composite of cobalt tetrakis(p-toyl) porphyrin substituted with a -COOH-group and Vulcan carbon (VC) exhibited a significant Faradaic efficiency of 94% for ammonia, along with 21% for HCOOH and 31% for CH_3COOH production in a neutral electrolyte solution. The experimental findings were well supported by the DFT calculations.

REFERENCES

1. Liao G, Smith Jr. RL, Guo H and Qi X. *Green Chem.* 2024; **26**: 11797-11831.
2. Kaur S, Garg K, Gupta D, Kafle A, Dharmender, Shukla V, Ahuja R and Nagaiah TC. *ACS Energy Lett.* 2025; **10**: 85-93.
3. Jiang H, Zhao P, Shen H, Yang S, Gao R, Guo Y, Cao Y, Zhang Q and Zhang H. *Small* 2024; **20**: 2304998.

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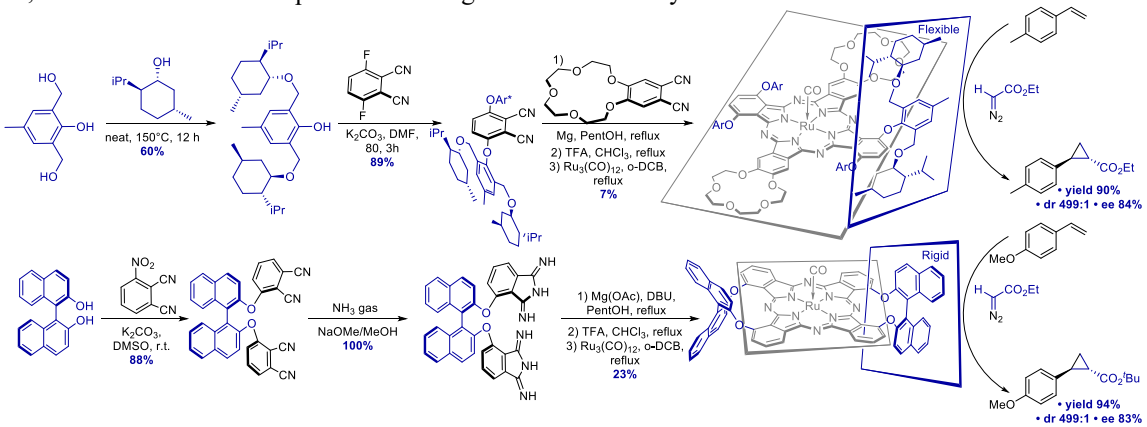


Novel architectures of chiral phthalocyanines for elaboration of asymmetric catalysts

Alexander A. Dmitrienko[a,b], Andrey P. Kroitor[a], Alexander A. Martynov[a], Yulia G. Gorbunova[a,c], Alexander B. Sorokin[d]

[a]*Frumkin Istitute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, Moscow, Russia*
[b]*Lomonosov Moscow State University, Moscow, Russia*
[c]*Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Scinces, Moscow, Russia*
[d]*Institut de Recherches sur la Catalyse et l'Environnement de Lyon, IRCELYON, Villeurbanne, France*

Enantioselective carbene transfer reactions mediated by chiral porphyrin complexes are powerful tools for the preparation of a wide range of valuable organic compounds. Metallophthalocyanines (MPcs), with their distinct electronic properties, can display catalytic reactivity that goes beyond porphyrins and often deliver higher turnover numbers. However, their use in asymmetric catalysis remains limited. Although many chiral MPcs are synthetically accessible, their chiral substituents are typically too far from the metal center and lie largely coplanar with the macrocycle. As a result, it is challenging to create a well-defined chiral environment near the metal center, which is an essential requirement for high enantioselectivity.



To tackle these obstacles, we developed two synthetic approaches to access catalytically-active ruthenium(II) complexes with well-defined chiral phthalocyanines. The first approach relies on cross-condensation between a bulky (−)-menthyl-derived phthalonitrile and a crown-functionalized phthalonitrile [1, 2], which enables efficient separation of positional isomers of "picket-fence" phthalocyanines bearing conformationally adaptive units. In the second approach, chirality is introduced via a BINOL-based bridging motif originally developed by N. Kobayashi [3, 4]. Both approaches afforded catalysts for asymmetric cyclopropanation with excellent diastereoselectivity and pronounced enantioselectivity. In addition, rigidity of the latter catalyst also enabled application of DFT modelling for interpretation of the observed selectivity.

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REFERENCES

1. A.P. Kroitor, A.A. Dmitrienko, *ACS Catal*., **2025**, 4984-5001.
2. A.P. Kroitor, A.A. Dmitrienko, *J. Porphyrins Phthalocyanines*, **2025**, 29, 726–735.
3. N. Kobayashi, *Chem. Commun.*, **1998**, 487-488.
4. A.A. Dmitrienko, A.P. Kroitor, *J. Catal*., **2025**, 452: 116443.

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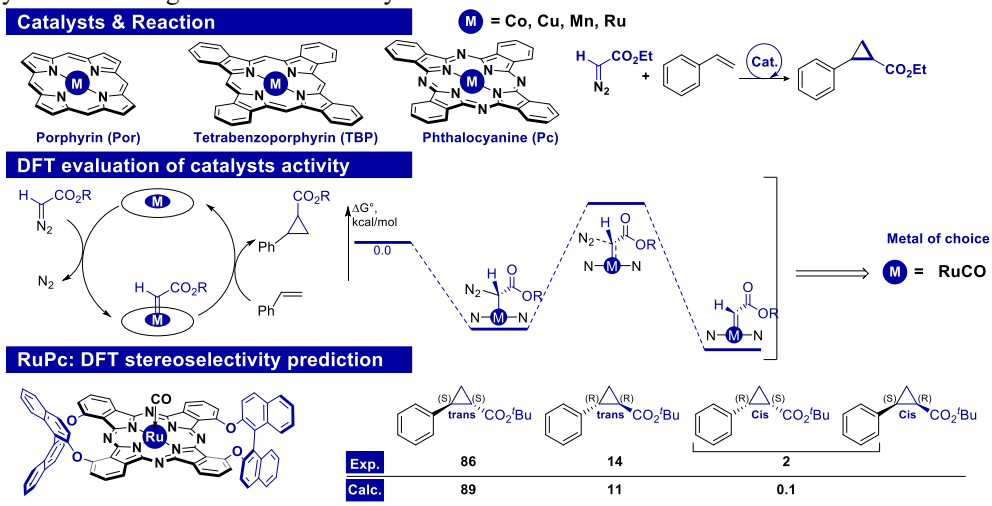
From screening to stereocontrol: DFT study of tetrapyrrolic catalysts for cyclopropanation

Alexander A. Dmitrienko[a,b], Andrey P. Kroitor[a], Yulia G. Gorbunova[a,c], Alexander B. Sorokin[d], Alexander A. Martynov[a]

[a]*Frumkin Istitute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, Moscow, Russia*
[b]*Lomonosov Moscow State University, Moscow, Russia*
[c]*Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Scinces, Moscow, Russia*
[d]*Institut de Recherches sur la Catalyse et l'Environnement de Lyon, IRCELYON, Villeurbanne, France*

Cyclopropanation via carbene transfer is an approach to versatile functionalized cyclopropanes, including pharmaceuticals and bioactive molecules. Although porphyrin complexes are widely employed as catalysts for this reaction, systematic comparison of their performance with other tetrapyrrolic platforms remains scarce. Here, we report a detailed DFT study of Ru(II), Mn(III), Co(II), and Cu(II) complexes supported by porphyrin, benzoporphyrin, and phthalocyanine ligands to identify the most active tetrapyrrolic scaffold.

DFT calculations indicate that trends in carbene formation barriers across ligands are not straightforward, whereas the nature of the metal center exerts a pronounced effect on reactivity and Ru complexes appear to be the most favorable choice. Based on these results, we focused on Ru phthalocyanine complexes as a particularly attractive system with a high turnover reactivity.



Thus, we have synthesized a chiral RuPc complex bearing binaphthyl substituents and evaluated its cyclopropanation performance [1]. To rationalize the stereoselectivity of asymmetric cyclopropanation, we performed DFT analysis of this system. The calculated cyclopropanation selectivity closely reproduces the experimental outcomes, accurately predicting both enantioselectivity (72% exp. vs 78% calc.) and diastereoselectivity (98:2 exp. vs 99:0.1 calc.). Finally, noncovalent interaction (NCI) analysis reveals key interactions that govern stereocontrol in this catalytic system.

Aknowledgment: This work has been supported by RSF, project № 25-13-00332.

REFERENCES

1. A.A. Dmitrienko, A.P. Kroitor, *J. Catal.*, **2025**, 452: 116443.

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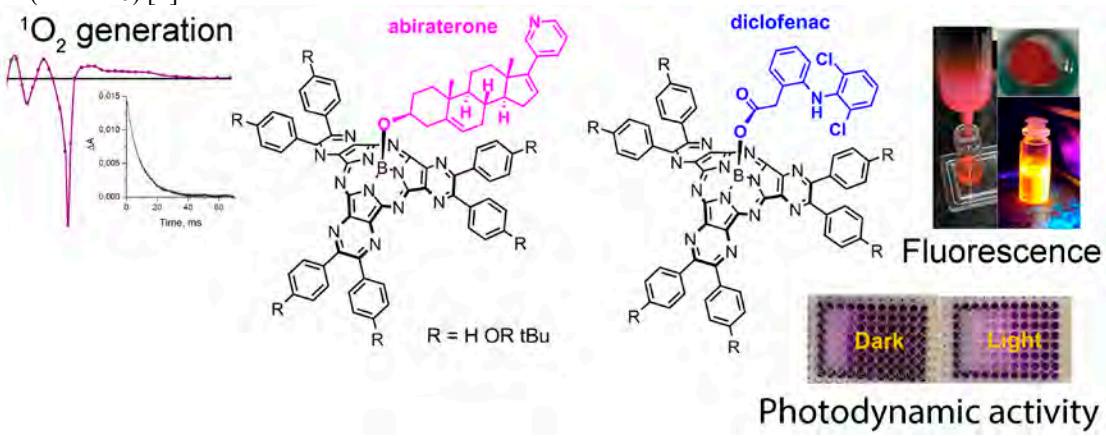


Subporphyrazine-drug hybrid photosensitizers containing diclofenac and abiraterone: synthesis, photophysical properties and photodynamic activity *in vitro*

Tatiana V. Dubinina[a], Roman O. Eremeev[a], Ivan D. Burtsev[b], Alina A. Markova[b], Vladimir A. Kuzmin[b]

[a]*Moscow State University, 1 Leninskie Gory, 119991 Moscow, Russia*
[b] *Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Kosygin st., 4, 119334 Moscow, Russia*

Novel tripyrrolic photosensitizers covalently linked to drug molecules were obtained by *post*-macrocyclization functionalization of pyrazine-fused boron subporphyrazines with diclofenac and abiraterone.
Optimization of the conditions of template cyclization and the purification procedure of initial chloro-substituted subporphyrazines allows increasing the yields by 5 times compared to literature data and obtaining sufficient quantities of pyrazinosubporphyrazines for the further introduction of axial molecules of drugs. The formation of an open-chain by-product of the macrocyclization reaction was detected.
The influence of the nature of the axial ligand, as well as peripheral groups, on the photophysical properties of subporphyrazines is shown. The results of flash photolysis showed the formation of triplet states. Bulky axial ligands (abiraterone, diclofenac) increase the contribution of vibrational relaxation of molecules, which is reflected in a decrease in fluorescence quantum yields and fluorescence lifetimes. The more rigid abiraterone does not reduce the fluorescence quantum yield as sharply as diclofenac. It was found that the introduction of a more rigid axial ligand abiraterone leads to an increase in the quantum yields of singlet oxygen to Φ=0.66 compared to the initial chlorine-substituted complexes. The opposite pattern was found for complexes containing diclofenac. In addition to bright fluorescence and efficient singlet oxygen generation, abiraterone-containing subporphyrazines demonstrated micromolar photodynamic activity *in vitro* and low dark cytotoxicity against a human colon cancer cell line (HCT116) [1].



The work was supported by Russian Science Foundation, grant number 23-73-10076.

REFERENCES

1.Eremeev R.O. et al. // Dyes and Pigments 241 (2025) 112868.

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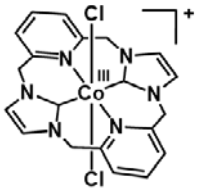


CO_2 Reduction Reaction Promoted by Macrocyclic Bis(NHC) Cobalt Complexes

Shunsuke Eguchi[a], **Chiwata Koshiro**[a], **Ken Sakai**[a], **Kosei Yamauchi**[a,b]

[a]*Department of Chemistry, Faculty of Science, Kyushu University, Nishi-ku, Fukuoka 819-0395, Japan.*
[b]*IAS, Kyushu University, Nishi-ku, Fukuoka 819-0395, Japan.*

Photochemical/electrochemical water reduction and CO_2 conversion to produce useful fuels have attracted considerable attention as a means of addressing the problems arising from global warming. Molecular catalysts are regarded as one of the most promising approaches due to their high tunability of electronic properties, which enables high activity and selectivity. Our group previously reported that a cobalt complex bearing a bis(NHC) macrocyclic ligand (**Co-NHC1**) shows excellent activity for hydrogen evolution from water [1,2]. Recently, we found that **Co-NHC1** and its derivative electrochemically convert CO_2 to high-density products under homogeneous electrocatalytic conditions. These results will be discussed in detail, including spectroelectrochemical measurements and computational analysis.



Co-NHC1

REFERENCES

1. K. Yamauchi, K. Kawano, K. Yatsuzuka, K. Kawamura, M. Kan, K. Sakai, *J. Am. Chem. Soc*., **2025**, *147*, 5602.
2. M. Kan, K. Yamauchi, K. Sakai *ChemRxiv.* **2025**, DOI: 10.26434/chemrxiv-2025-hwww9.

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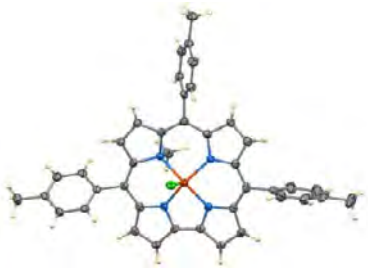


Synthesis of Iron-N-methyl corroles

Alessia Fata,[a] Sara Nardis,[a] Francesco Pizzoli,[a] Frank R. Fronczek,[b] Kevin M. Smith,[b] and Roberto Paolesse[a]

[a]*Department of Chemical Sciences and Technologies, University of Rome Tor Vergata, via della Ricerca Scientifica, 00133 Rome, Italy*
[b]*Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana 70803, United States*

Within the porphyrinoid family, corroles constitute a highly versatile group of compounds, owing to their distinctive chemical properties. This versatility stems from their exceptional coordination flexibility, which enables the incorporation of a wide range of metals and supports the concept of the Periodic Table of Metallocorroles. [1] Furthermore, their distinctive reactivity and photophysical properties enable their application as sensing materials in chemical sensors for optical, electrochemical, and conductometric transducers. [2] Their catalytic activity has also been investigated and reported in several publications; iron corroles, for instance, are more selective catalysts than porphyrin analogues for the aziridination of olefins [3] and specific functionalizations on their *meso* positions can be explored for their application in electrocatalysis.[4] Furthermore, the use of metallocorroles resulted in a very powerful cooperative catalytic system for CO_2 fixation with epoxides. [5] This work focuses on the synthesis and characterization of iron meso-arylcorrole complexes and their N-methylated analogues, with particular attention to their electrochemical properties. The synthesis of these N-substituted macrocycles is of significant interest, as it provides a uniquely appealing platform owing to their underexplored chirality in catalysis. To evaluate their potential in this context, the initial investigations into the complexes' catalytic properties are carried out.



REFERENCES

1. S. Nardis, F. Mandoj, M. Stefanelli, R. Paolesse, *Coord. Chem. Rev.*, 2019, *388*, 360–405.
2. R. Paolesse, S. Nardis, D. Monti, M. Stefanelli, and C. Di Natale, *Chem. Rev.*, 2017, *117*, 2517-2583.
3. L. Simkhovich, Z. Gross, *Tetrahedron Lett.*, 2001, *42*, 8089–8092.
4. W. Sinha, A. Mahammed, N. Fridman, Z. Gross, *ACS Catal*., 2020, *10*, 3764−3772.
5. M. Tiffner, S. Gonglach, M. Haas, W. Schçfberger, M. Waser, *Chem. Asian J.,* 2017, *12*, 1048–1051.

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Alcoholysis of Perfluorinated Boron(III) Subphthalocyanine Leading to Diazatripyrrins (DATRIPYs)

Alina M. Fazlyeva[a], Ivan A. Skvortsov[a], Pavel A. Stuzhin[a]

[a]*Research Institute of Macroheterocyclic Compounds, Ivanovo State University of Chemistry and Technology, RF-153000, Ivanovo, Russia*

Perfluorinated subphthalocyanine is widely studied as an acceptor material for organic electronics [1], so the question of its stability is of great importance. It was noticed that the addition of bases or nucleophilic molecules (cyanide, amino acid) [2, 3] to its solution can lead to some irreversible spectral changes, but the reason remained unexplained. Previously, we found that boron(III) subphthalocyanine analogs with electron-withdrawing moieties (pyrazine fused and/or perhalogenated) undergo hydrolytic cleavage of the macrocycle and deborylation in the presence of water [4]. This results in the formation of non-cyclic aza-bridged *tris*-isoindoles, which are fused derivatives of 5,10-diazatripyrrins (DATRIPY). This reaction easily occurs for perhalogenated and/or aza-substituted boron(III) subphthalocyanine analogs, yielding the pyrazine-fused 14-amino-5,10-diazatripyrrin-1-one existing according to X-ray diffraction analysis in an *S*-shaped conformation stabilized by two intramolecular hydrogen bonds between the pyrrole and the pyrrolenine and pyrazine. A similar reaction was also observed for perfluorinated subphthalocyanine (F_{12}sPcBBr) in acetone containing water.

In this work, we studied the spectral behaviour of F_{12}sPcBBr in alcohols and observed the macrocycle cleavage and deborylation leading to an open tris-isoindole derivative with terminal amino and alkoxy groups and two bridging *meso*-nitrogens (**Fig. 1**). The products were characterized by FTIR, MALDI-TOF and NMR spectroscopy and the photophysical properties of the compounds have been investigated. *E*/*Z* isomerism of the bonds formed by the meso-nitrogen bridge and possible reaction mechanisms are also discussed.

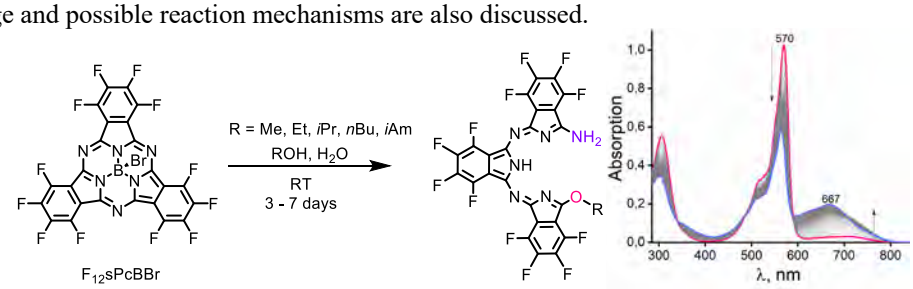


Fig. 1. Synthesis of diazatripyrrins from F_{12}sPcBBr

The support from the Russian Science Foundation (grant 25-73-20126) is gratefully acknowledged.

REFERENCES

1. Morse, G. E., Helander, M. G., Maka, J. F., Lu, Z. H., Bender, T. P. *ACS Applied Materials & Interfaces*, 2010, 2(7), 1934-1944.
2. Demuth, J., Gallego, L., Kozlikova, M., Machacek, M., Kucera, R., Torres, T., Novakova, V. *Journal of Medicinal Chemistry*, 2021, 64(23), 17436-17447.
3. Palomares, E., Martínez-Díaz, M. V., Torres, T., Coronado, E. *Advanced Functional Materials*, 2006, 16(9), 1166-1170.
4. Fazlyeva, A. M., Skvortsov, I. A., Somov, N. V., Stuzhin, P. A. *Inorganic Chemistry*, 2025, 64(38), 19197-19206.

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Coumarin-Annulated Subporphyrazine: Synthesis and Photophysical Properties

Karina R. Romanova[a], Alina M. Fazlyeva[a], Ivan A. Skvortsov[a], Pavel A. Stuzhin[a]

[a]*Research Institute of Macroheterocyclic Compounds, Ivanovo State University of Chemistry and Technology, RF-153000, Ivanovo, Russia*

Subphthalocyanines (sPcs) are well-known photosensitizers capable of generating reactive oxygen species, while hydroxy-substituted coumarins are natural fluorophores exhibiting intense fluorescence [1,2]. Unsymmetrical subphthalocyanines have been previously obtained and are of considerable interest, since the combination of different annelated fragments in a single macrocycle allows tuning of their photophysical properties. It was shown for a series of unsymmetrical subporphyrazines that replacement of fluorinated benzene rings with pyrazine fragments leads to a hypsochromic shift of the Q-band and a decrease in the fluorescence quantum yield compared to the starting perfluorinated subphthalocyanine F_{12}sPc [3]. However, subporphyrazines containing pyrazinocoumarin fragments on the periphery have not been obtained so far, and their photophysical properties remain unexplored.

In this work, we have studied the preparation of the coumarine-fused dinitrile precursors from halogenated derivatives by aromatic nucleophilic substitution. Their reactivity in cyclotrimerization in the presence of boron(III) halides, leading to corresponding subporphyrazines, was investigated. Thus, new coumarin-substituted pyrazine-2,3-caarbonotrile was then used for the preparation of an unsymmetrical pyrazino-subporphyrazine annelated with a pyrazinocoumarin fragment.

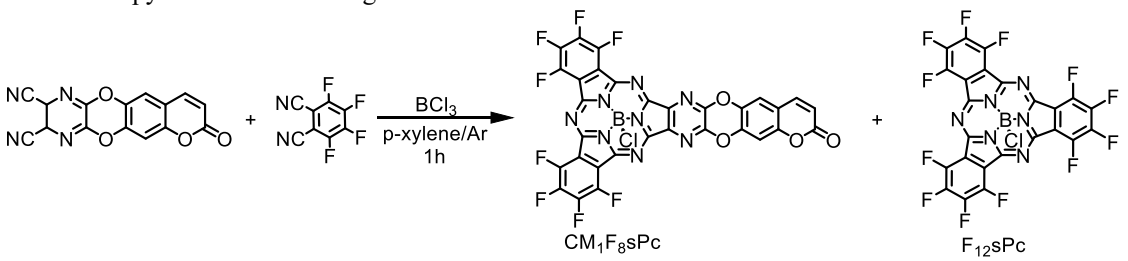


Fig. 1. Synthesis of coumarin-annelated pyrazino-subporphyrazine.

The obtained compounds were characterized by MALDI-TOF mass spectrometry, NMR and IR spectroscopy. The photophysical properties of the new subporphyrazine were investigated in comparison with F_{12}sPc. The possibilities of obtaining other coumarin derivatives of subphthalocyanine are also being discussed.

The work was carried out with the financial support of the Russian Science Foundation.

REFERENCES

1. Ortega-Forte, E., Rovira, A., Gandioso, A., Bonelli, J., Bosch, M., Ruiz, J., Marchán, V. *Journal of Medicinal Chemistry*, 2021, 64(23), 17209-17220.
2. Zhao, N., Li, Y., Yin, W., Zhuang, J., Jia, Q., Wang, Z., Li, N. *ACS Applied Materials & Interfaces*, 2019, 12(2), 2076-2086.
3. Kovkova, U. P., Skvortsov, I. A., Khodov, I. A., Efimov, S. V., Zhabanov, Y. A., Somov, N. V., Liang, X., Pakhomov, G. L., Stuzhin, P. A. *Journal of Porphyrins and Phthalocyanines*, 2023, 27, 1-14.

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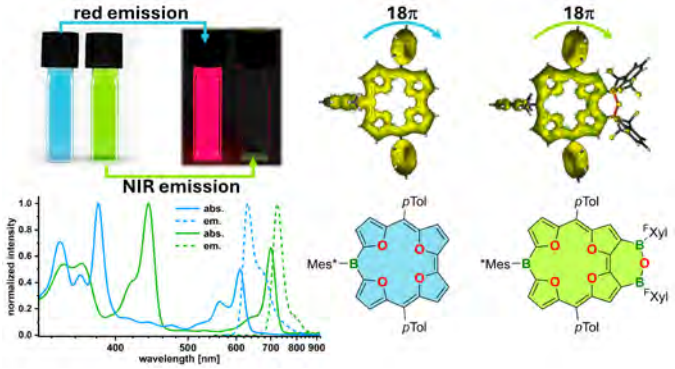


Aromatic Boratetraoxacorroles: A Mirror Image of Antiaromatic Boracorrole

Jonas Fehler, Lukas Swoboda, Vivien Schütz, Holger Helten*

Julius-Maximilians-Universität Würzburg, Institute of Inorganic Chemistry and Institute for Sustainable Chemistry & Catalysis with Boron (ICB), Am Hubland, 97074 Würzburg, Germany
holger.helten@uni-wuerzburg.de

Corroles are contracted porphyrin analogues lacking one *meso*-carbon atom. While corroles and their skeletal variants are well studied, direct incorporation of heteroatoms into the corrole's π-aromatic framework remains rare, despite its strong influence on electronic structure, coordination ability, and spectroscopic properties.[1] Replacement of the 10-*meso*-carbon atom by a heteroatom (N, O, S, P, or Se) affords 10-heterocorroles whose global aromaticity, governed by π-conjugation through the heteroatom, contrasts with the antiaromatic 10-metalla- and 10-boracorroles.[2] Boron, owing to its electron deficiency, coordination flexibility, and ability to modulate π-conjugation and aromaticity, is an attractive heteroatom for π-conjugated macrocycles, as we recently demonstrated with a series of (expanded) porphyrinoids.[3] Motivated by these considerations, we sought to introduce boron into furan-based corrole frameworks, a structural motif previously unreported. Herein, we describe the synthesis of the first 10-boratetraoxacorroles, together with an oxadiborepin-appended derivative,[4] which exhibit intense visible absorption, enhanced visible-to-near-infrared photoluminescence, and versatile electrochemical behavior.[5]



REFERENCES

1. a) C. D. Natale, C. P. Gros, R. Paolesse, *Chem. Soc. Rev.* **2022**, *51*, 1277; b) R. Orłowski, D. Gryko, D. T. Gryko, *Chem. Rev.* **2017**, *117*, 3102.
2. a) K. Miwa, T. Yokota, Q. Wang, T. Sakurai, H. Fliegl, D. Sundholm, H. Shinokubo, *J. Am. Chem. Soc*. **2024**, *146*, 1396; b) H. Omori, H. Shinokubo, *Organometallics* **2019**, *38*, 2878.
3. a) L. Swoboda, J. Klopf, M. Fest, A. Friedrich, M. Buckel, I. Krummenacher, H. Braunschweig. B. Engels, H. Helten, *J. Am. Chem. Soc*. **2026**, *148*, 2639; b) L. Swoboda, J. Klopf, M. Buckel, B. Engels, H. Helten, *J. Am. Chem. Soc*. **2025**, *147*, 10629; c) M. Buckel, J. Klopf, J. S. Schneider, A. Lik, N. A. Riensch, I. Krummenacher, H. Braunschweig, B. Engels, H. Helten, *Nat. Commun.* **2025**, *16*, 1775.
4. a) J. Bachmann, A. Helbig, M. Crumbach, I. Krummenacher, H. Braunschweig, H. Helten, *Chem. Eur. J.* **2022**, *28*, e202202455; b) M. Crumbach, J. Bachmann, L. Fritze, A. Helbig, I. Krummenacher, H. Braunschweig, H. Helten, *Angew. Chem. Int. Ed.* **2021**, *60*, 9290.
5. J. Fehler, L. Swoboda, V. Schütz, H. Helten, *manuscript in preparation.*

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Affecting the Properties of the Parent-Corrole Cobalt Complexes by Axial Ligands

Marcelo Fernandez de la Mora[a], Irena Saltsman[a], Shachar Fite[a], Natalia Fridman[a], Atif Mahammed[a], and Zeev Gross[a]

[a]*Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, Haifa, Israel*

While corroles were first discovered in 1964 by Kay and Johnson, access to the unsubstituted parent corrole remained elusive due to the macrocycle's tendency to undergo decomposition when exposed to light and air.[1] This challenge was resolved in 2021 by isolating a variety of the much more stable metal complexes, (cor)M(L), with M = Ga, Co, Re, Mo, and Mn, and L standing for a variety of axial ligands.[2] As this stability particularly applies to cobalt(III) complexes, an opportunity arose to study how axial ligands govern fundamental properties of corroles. This goal was achieved by preparing a series of (cor)Co(L)$_2$ complexes, where L consists of pyridine, substituted pyridines, and 1-methylimidazole. All the complexes were examined *via* X-ray crystallography (Figure 1), UV-Vis and ^{1}H-NMR. These studies revealed small but significant differences in the Co-N axial bond lengths, modest changes in their electronic spectra, and substantial variations in their ^{1}H-NMR chemical shifts. DFT calculations focusing on these properties provided insight in how the different phenomena are related to each other.

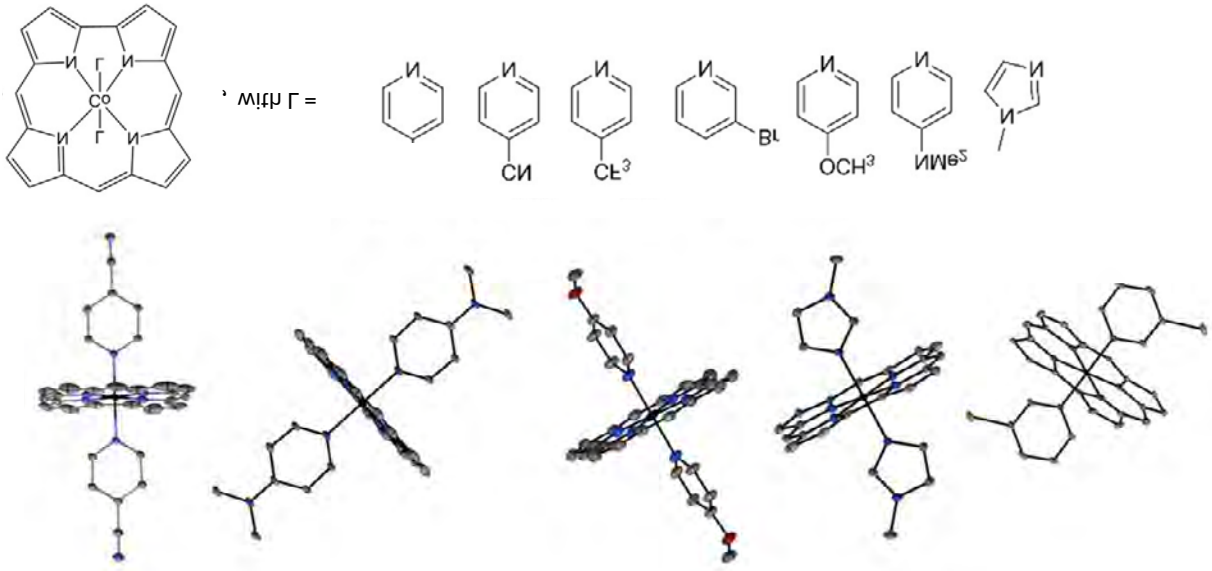


Figure 1. The cobalt(III) complexes of the parent corrole and X-ray structures corresponding to five of them.

REFERENCES

1. Johnson, A. W.; Kay, I. T. 306. Corroles. Part I. Synthesis. *J. Chem. Soc.* **1965**, No. 0, 1620–1629.
2. A. Kumar, P. Yadav, M. Majdoub, I. Saltsman, N. Fridman, S. Kumar, A. Kumar, A. Mahammed, Z. Gross. Corroles: The Hitherto Elusive Parent Macrocycle and its Metal Complexes. *Angew. Chem. Int. Ed.* **2021**, *60*, 25097.

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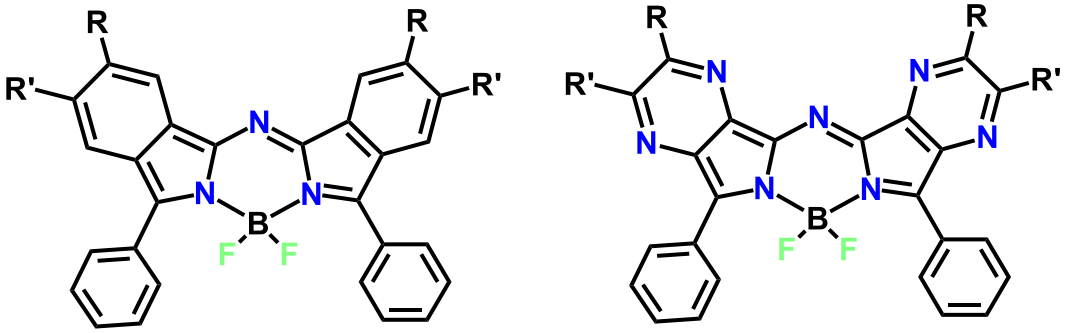


Aza-BODIPY Analogues: Effect of Substitutents in the Fused Rings (Benzene|Pyrazine) on *Z,E*-Isomerism, Spectral and Electrochemical Properties

Daniil N. FInogenov[a], Alexander A. Kalyagin[b], Dominika Yu. Parfyonova[a], Pavel A. Stuzhin[a]

[a] *Research Institute of Macroheterocyclic Compounds, Ivanovo State University of Chemistry and Technology, Sheremet'evskiy av. 7, Ivanovo, 153000*
[b] *Institute of Solution Chemistry, Russian Academy of Sciences, Academic St. 1, Ivanovo, 153045*

Aza-BODIPY today is one of the "hot theme" of dyes chemistry. Introsuction of the nitrogen atom (–N=) instead of the methene –CR= bridge leads to significant changing of properties. The considerable interest in aza-BODIPYs stems from their extensive functionalization potential, which enables precise control over their spectral and luminescent properties [1]. The presence of a nitrogen atom at the *meso*-position enhances intersystem crossing, leading to a higher quantum yield of the triplet state, all while retaining their fluorescent characteristics. Despite this, fused-ring aza-BODIPY derivatives remain poorly understood. Earlier investigations focused predominantly on modifying the bottom aryl substituent, with the influence of the fused rings themselves receiving little attention [2]. A reported pyrazine-annelated aza-BODIPY, for example, was studied only for its sensitivity to ammonium ions, leaving other key photophysical characteristics unexplored [3]. We show that presence of pyrazine rings in the aza-dipyrromethene fragment can induce *Z,E*-isomerism [4,5].



In this work, we present a series of compounds bearing various alkyl, aryl, and aryloxy substituents into both the pyrazine and benzene rings. Their key photophysical properties were investigated, revealing a clear dependence on both the nature of the substituents and the annulation pattern. Furthermore, electrochemical studies demonstrated that aza-substitution within the annulated fragment induces a substantial shift in redox potentials and significantly alters the frontier molecular orbital energies.

This work was supported by Russian Science Foundation (grant RSF 25-73-20126)

REFERENCES

[1] M. Kaur, et al, *Coordination Chemistry Reviews*, **2024**, *498*, 215428.
[2] R. Gresser, et al, *Chem. Eur. J*. **2011**, *17*, 2939–2947
[3] H. Liu, et al, *Chem. Commun*. **2011**, *47*, 12092–12094
[4] A.M. Fazlyeva, et al, *Inorg. Chem.*, **2025**, *64* (38), 19197-19206
[5] D.N. Finogenov, et al. *Macroheterocycles*, **2026**

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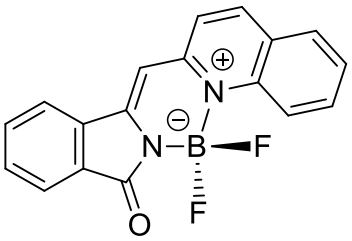


Benzo-, pyridino- and pyrazino-annulated unsymmetrical BODIPY analogues: effect of aza-substitution on physicochemical properties

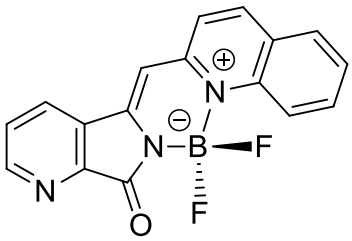
Nikolay E. Galanin[a], Daniil N. Finogenov[a], Roman A. Novikov[a], Taisia A. Rumyantseva[a], Pavel A. Stuzhin[a]

[a] *Research Institute of Macroheterocyclic Compounds, Ivanovo State University of Chemistry and Technology, Sheremet'evskiy av. 7, Ivanovo, 153000*

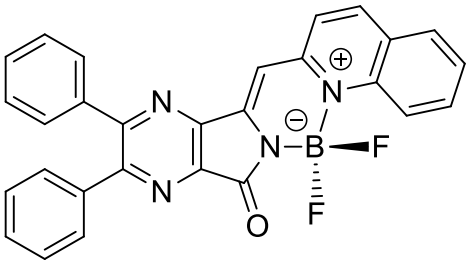
Unsymmetrical analogs of BODIPY can exhibit large Stokes shifts and intense solid-state emission. However, their synthesis is often a multistep procedure requiring the use of expensive reagents. In this regard, derivatives of keto-pyrrolyl-quinolines [1] are of interest; their synthesis is highly technological and involves the condensation of quinaldine with imides of aromatic *o*-dicarboxylic acids followed by complexation with boron [2]. We synthesized a series of complexes (**1–3**) characterized by varying acceptor properties of the annulated rings [3, 4].



1



2



3

We discuss effects of aza-substitution in the benzene ring of isoindolone unit on the electronic structure, spectral and luminescent properties in solutions and the solid state, and solvatochromic effects. Based on quantum-chemical calculations and electrochemical studies, it was established that all the obtained complexes have low LUMO energies and are promising for further research as acceptors for the fabrication of multilayer OLEDs.

This work was supported by Russian Science Foundation (grant RSF 25-73-20126)

REFERENCES

1. Y. Zhou, Y. Xiao, D. Li, M. Fu, X. Qian, *J. Org. Chem.,* **2008**, *73*, 1571–1574.
2. A.A. Nabasov, T.A. Rumyantseva, A.I. Koptyaev, N.E. Galanin, *Dyes Pigm.*, **2023**, *219*, 111523.
3. A.A. Nabasov, A.I. Koptyaev, S.D. Usoltsev, T.A. Rumyantseva, N.E. Galanin, *Macroheterocycles*, **2022**, *15*, 128–132.
4. T.A. Rumyantseva, R.A. Novikov, N.E. Galanin, A.A. Kalyagin, D.N. Finogenov, P.A. Stuzhin, *J. Mol. Struct.*, **2026**, *357*, 145224.

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Synthesis of Butadiyne-Linked Cyclic Pyrrolopyrrole aza-BODIPY Oligomers via Platinum Coordination

Shuhei Fukami, Takanori Iwasaki, and Soji Shimizu

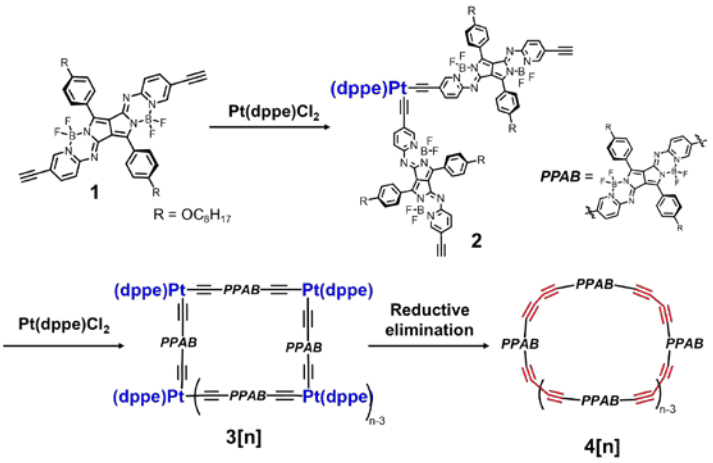
Department of Applied Chemistry, Graduate School of Engineering, Kyushu University, Fukuoka 819-0395, Japan (fukami.shuhei.782@s.kyushu-u.ac.jp)

Pyrrolopyrrole aza-BODIPY (PPAB), a dimeric aza-BODIPY structure comprising a diketopyrrolopyrrole (DPP) unit, exhibits intense absorption and emission in the visible and near-infrared regions [1]. In our previous work, we successfully controlled the optical properties by changing the aryl groups on the DPP unit and the heteroaromatic ring units. Recently, we also achieved the synthesis of chiral PPAB in a one-pot manner from DPP bearing *o*-anisyl substituents via ether cleavage and chelation of the liberated oxygen atoms to boron atoms, forming the *B*,*O*-chelated PPAB [2]. Due to the absence of the inversion center, the *syn*-type isomer of *B*,*O*-chelated PPAB, in which the axial ligands point in the same direction, exhibited circular dichroism (CD) and circularly polarized luminescence (CPL). However, the dissymmetry factor (*g*-value) was as low as 10^{-4}.

In recent years, it has been reported that cyclic organic molecules exhibit higher *g*-values than regular organic chromophores [3]. The high *g*-values were explained by the cancellation of the transition electric dipole moments along the circumferential direction and by the rather enhanced transition magnetic dipole moments as the ring size increased.

zIn this study, to improve *g*-values of PPAB chromophores, we attempted to synthesize a butadiyne-linked cyclic oligomer (**4[n]**) using PPAB. To construct a cyclic structure, butadiyne was used as the linker, and the cyclization reaction was carried out based on the method developed in the synthesis of butadiyne-bridged cyclic oligothiophene reported by Bäuerle *et al* [4]. As a precursor of the target molecule, a platinum-bridged PPAB dimer (**2**) was synthesized from ethynyl-substituted PPAB (**1**) using $PtCl_2$(dppe). Then, **2** was reacted again with $PtCl_2$(dppe) to synthesize a platinum-bridged cyclic PPAB oligomer (**3[n]**). Finally, reductive elimination was examined under illuminating UV light in the presence of iodine.

In this poster presentation, the synthesis of **2** and **3[n]**, and the progress in the synthesis of **4[n]** will be reported.



Scheme. Synthetic route of butadiyne-linked cyclic-PPAB oligomer (**4[n]**)

REFERENCES

1. Shimizu S, *Chem. Commun*. 2019; 55: 8722.
2. Fukami S, Mori S, Harada T, Shimizu S, *Chem. Commun*. 2024; 60: 6170
3. Saito S, Yoshii A, Takahashi S, Furumi S, Takeuchi M, Isobe H, *PNAS* 2017; 114: 13097.
4. Fuhrmann G, Debaerdemaekerb T, Bäuerle P, *Chem. Commun*. 2003; 948.

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Development of Quinoidal Conjugated Molecules Based on Isobenzoheterole Units

Minamo Furuta[a], **Keitaro Yamamoto**[a], **Mitsuaki Yamauchi**[a], **Hiroko Yamada**[a]

[a]*Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*

Quinoidal conjugated molecules have been extensively studied as electron-transporting organic semiconductors owing to their high electron affinity and strong intermolecular interactions. They also exhibit sharp long-wavelength absorption stemming from their narrow HOMO–LUMO energy gaps. Although quinoidal molecules intrinsically exhibit high oscillator strengths, their emission properties have rarely been reported, presumably due to enhanced nonradiative decay associated with their diradical character. It is expected that imparting emissive properties to quinoidal molecules will enable their use in next-generation optoelectronic devices, such as organic light-emitting transistors (OLETs). In our previous studies, we developed quinoidal oligothiophenes incorporating isothianaphthene units and demonstrated that their diradical character can be effectively controlled [1]. Furthermore, we found that increasing the number of isothianaphthene units enhances fluorescence [2].

In this study, we designed quinoidal molecules based on isobenzoheterole units to explore their emissive properties. The molecular design systematically varies the conjugation length and heteroatoms (sulfur and oxygen) to evaluate the structure–property relationships (Fig. 1a). Notably, isobenzofuran-type quinoids represent a previously unexplored molecular framework, where the furan unit is expected to enhance molecular planarity and quinoidal character. To synthesize the target molecules, we employed a precursor strategy based on retro-Diels–Alder reactions to generate isobenzoheterole units. To date, compound **1** has been synthesized and exhibits distinct long-wavelength fluorescence even at room temperature (Fig. 1b).

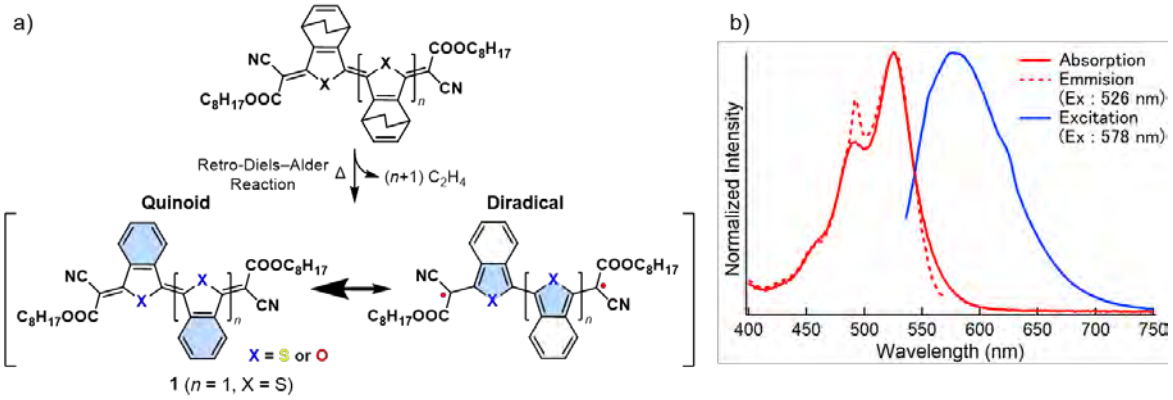


Figure 1. a) Molecular structures and synthetic strategy in this study. b) Absorption, emission, and excitation spectra of compound **1**.

REFERENCES

1. Cross-conjugated isothianaphthene quinoids: a versatile strategy for controlling electronic structure, K. Yamamoto, S. M. Quintero, S. Jinnai, E. Jeong, K. Matsuo, M. Suzuki, H. Yamada, J. Casado, Y. Ie, *J. Mater. Chem. C* **2022**, *10*, 4424–4433.
2. Oligoene and cyanine features of tetracyano quinoidal oligothiophenes, S. M. Quintero, J. L. Zafra, K. Yamamoto, Y. Aso, Y. Ie, J. Casado, *J. Mater. Chem. C* **2021**, *9*, 10727–10740.

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Porphycenes bearing electron-withdrawing groups: synthesis, spectroscopy, photophysics, and photostability

Agnieszka Gajewska, Aleksander Gorski, Jacek Waluk

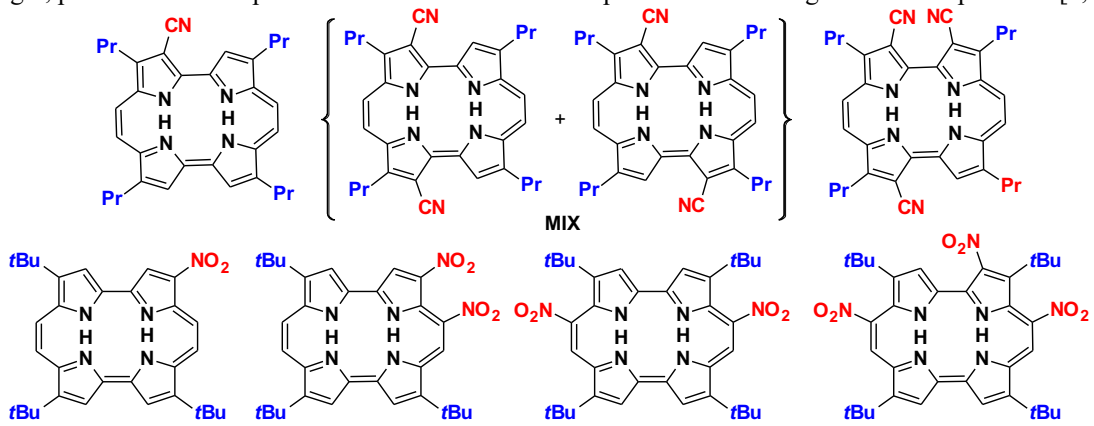
Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, Warsaw, Poland

Porphycenes are hydrogen-bonded macrocycles whose excited-state dynamics are highly sensitive to substitution pattern and structural distortion [1]. Electron-withdrawing groups are known to modify nonradiative deactivation pathways and enhance photostability, yet the influence of their number and position within the porphycene framework remains insufficiently understood [2,3].

Here we present systematic studies of two series of electron-withdrawing substituted porphycenes: β′-cyano derivatives of 2,7,12,17-tetrapropylporphycene (mono-, di-, and tri-substituted) and nitro-functionalized 2,7,12,17-tetra-tert-butylporphycenes with varied substitution patterns. This design enables controlled tuning of electronic effects while simultaneously modulating steric constraints within the macrocycle.

Cyano-substituted tetrapropyl derivatives retain strong fluorescence together with enhanced photostability, making them promising candidates for imaging applications. In contrast, tetra-*tert*-butyl porphycenes bearing two or more nitro groups exhibit strongly suppressed emission in fluid solution due to efficient nonradiative decay; however, fluorescence is partially restored in viscous or rigid environments, indicating their potential as photostable viscosity-responsive probes.

By varying both the number and position of electron-withdrawing substituents, we establish a direct relationship between substitution pattern, photostability, and viscosity-dependent emission behaviour. These results demonstrate that rational electronic and/or steric modification of the porphycene scaffold enables the design of either bright, photostable fluorophores or environment-sensitive probes within a single molecular platform [1,2].



REFERENCES

[1] Gil, M.; Dobkowski, J.; Wiosna-Sałyga, G.; Urbańska, N.; Fita, P.; Radzewicz, C.; Pietraszkiewicz, M.; Borowicz, P.; Marks, D.; Glasbeek, M.; Waluk, J., *J. Am. Chem. Soc.*, **2010**, 132, 13472–13485.

[2] Mbakara, I.; Gajewska, A.; Listkowski, A.; Kijak, M.; Nawara, K.; Kumpulainen, T.; Vauthey, E.; Waluk, J., *Phys. Chem. Chem. Phys.*, **2022**, 24, 29655–29666.

[3] Gajewska, A.; Mbakara, I.; Waluk, J., *J. Porphyrins Phthalocyanines*, **2023**, 27, 563–568.

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Aromaticity Flip-Flop: Spectroscopic Insights into Pyridine-Fused Oxacorrole Dimers Across Their Redox States

Aleksandra Gałązka,[a] Qin Liu,[b] Sha Li,[b] Guoru Chen,[b] Xiaofang Li,[b] Michał J. Białek,[a] and Piotr J. Chmielewski[a]

[a] *Department of Chemistry, University of Wrocław, 14 F. Joliot-Curie, Wrocław, 50 383, Poland.*
[b] *Key Laboratory of Theoretical Organic Chemistry and Functional Molecules, Ministry of Education, School of Chemistry and Chemical Engineering Hunan University of Science and Technology Xiangtan, Hunan 411201, China.*

Porphyrinoids encompass a wide range of structures, including porphyrins, corroles, and expanded macrocycles, with tunable aromatic, non-aromatic, or antiaromatic properties dictated by their structure and electron delocalisation. Linking porphyrinoid units to form dimers offers a strategy for modulating their properties, while fused architectures enable particularly strong inter-subunit electronic coupling.[1-5] Pyridine-fused bis(10-oxacorroles) represent a novel class of such systems, in which a heteroaromatic bridge ensures efficient conjugation and redox-responsive communication between the two macrocyclic halves.[6] In this study, we report a detailed spectroscopic and theoretical characterisation of their neutral, monocationic, and dicationic states. Nuclear magnetic resonance, UV-Vis-NIR and electron paramagnetic resonance spectroscopy, supported by quantum-chemical calculations, reveal a striking "aromaticity flip-flop" behaviour: the redistribution of π-electron delocalisation upon sequential oxidation leads to a reversible switch between locally aromatic, globally non-aromatic, and fully delocalised states. This modulation strongly affects optical and magnetic properties, enabling pronounced near-infrared absorption features that extend into the readily accessible NIR-III window. Such behaviour highlights the potential of pyridine-fused oxacorrole dimers as redox-controllable chromophores for molecular electronics and photonic applications.

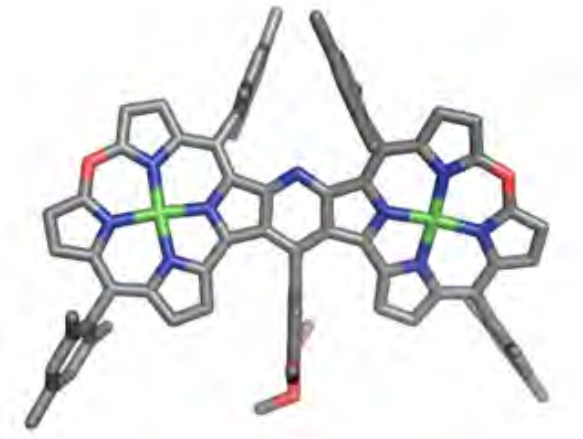


Figure 1. Exemplary structure of one of the oxacorrole dimers obtained.

REFERENCES

1. S. Cho, J. M. Lim, S. Hiroto, P. Kim, H. Shinokubo, A. Osuka, D. Kim, J. Am. Chem. Soc. 2009, 131, 6412.
2. B. Liu, X. Li, M. Stępień, P. J. Chmielewski, Chem. Eur. J. 2015, 21, 7790.
3. X. Li, Y. Meng, P. Yi, M. Stępień, P. J. Chmielewski, Angew. Chem. Int. Ed. 2017, 56, 10810.
4. K. Wang, S. Ito, D. Ren, Shimizu, N. Fukui, R. Kishi, Q. Liu, A. Osuka, J. Song, H. Shinokubo, Angew. Chem. Int. Ed. 2024, 63, e202401233.
5. S. Li, S. Zhang, X. Li, O. Smaga, K. Szydełko, M. Pawlicki, P. J. Chmielewski, Adv. Sci. 2025, 12, 2416223.
6. Q. Liu, S. Li, G. Chen, X. Li, A. Gałązka, M. J. Białek, P. J. Chmielewski, Chem. Eur. J., 2025, 31: e202501085.

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Pyridine Functionalized Aza-BODIPY for use as Electron Acceptors

Edward Gilbreth[a], David Blank[b], Victor Nemykin[a]

[a]*Department of Chemistry, University of Tennessee – Knoxville, TN, USA*
[b]*Department of Chemistry, University of Minnesota – Minneapolis, MN, USA*

Aza-boron-dipyrromethene (aza-BODIPY) is a versatile chromophore known for its ease of synthesis, chemical stability, and chemical tunability. The presence of the *meso* nitrogen makes the aza-BODIPY platform a potential electron acceptor in dye-sensitized solar cells. In this project, we synthesized novel tetraphenyl aza-BODIPY derivatives and coupled them with pyridine via click chemistry. These compounds were characterized via UV-Vis and fluorescence spectroscopy, as well as HRMS, HNMR, CNMR, HSQC, and COSY NMR techniques. These were then titrated with zinc perfluorotetraphenyl porphyrin to investigate their potential as a donor-acceptor complex with the aza-BODIPY acting as the electron acceptor. The binding constants of these complexes were calculated by absorbance and fluorescence titrations, and they were further characterized via CV, DPV, and spectrochemical methods.

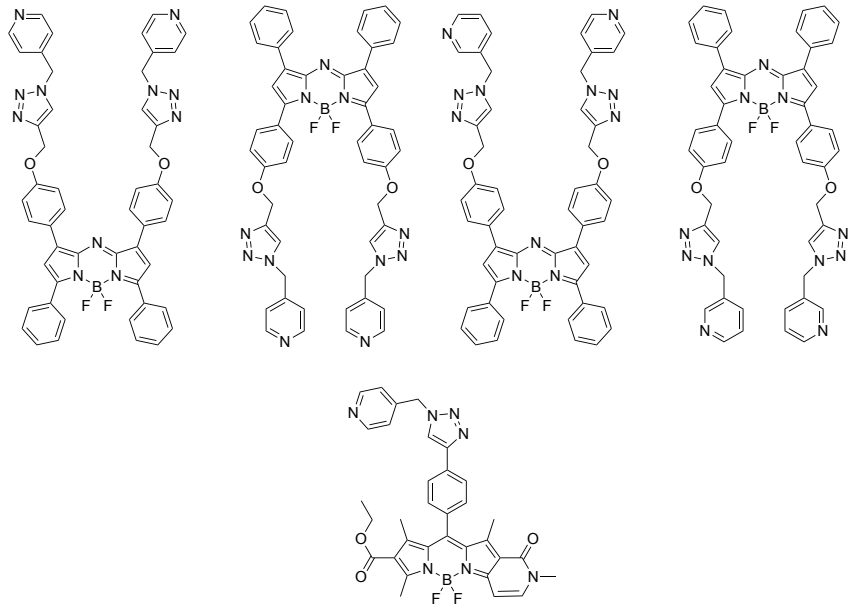


Figure 1. Structures of the pyridine-coupled BODIPY aza-BODIPY derivatives.

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Tuning Molecular Light Emission Through Atomic-Scale Control of the Local Environment

Thiago G.L. Brito[1], Daniel Arribas[1], Sofia Canola[2], Klaus Kuhnke[1], Tomáš Neuman[2], Anna Rosławska[1]

[1] Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany
[2]Institute of Physics, Czech Academy of Sciences, 16200 Prague, Czech Republic

Intermolecular distances, adsorption sites, and configurations define a molecule's local environment, but their combined effect on single-molecule emission across different excitation pathways remains unclear. In this study, we measure the singlet emission of zinc phthalocyanine (ZnPc) on NaCl/Ag(111) and introduce platinum phthalocyanine (PtPc) as both a controlled perturbation of the local environment and a probe of ZnPc emission via resonant energy transfer (RET). All measurements were performed using scanning tunneling microscopy induced luminescence (STML) and tip-enhanced photoluminescence (TEPL). By systematically tuning intermolecular distances, restricting molecular rotational motion, and comparing direct electrical excitation with RET-driven and photon excitations, we reveal previously inaccessible regimes of ZnPc singlet emission, including neutral exciton-libron coupling. We further disentangle the environmental factors that influence emission spectra, demonstrating how the local environment actively shapes the optical response of single molecules.

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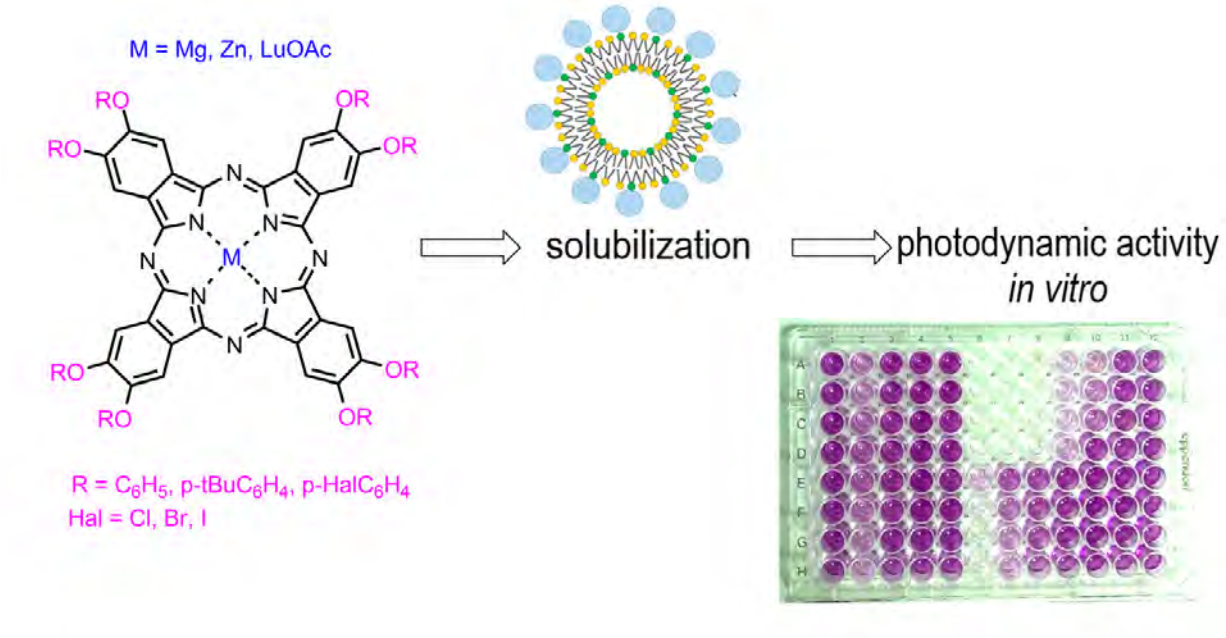
Aryloxy-substituted phthalocyanunes: synthesis, photophysical properties and *in vitro* photodynamic activity

Elena A. Gorbunova[a], Alina S. Agranat[a], Andrey V. Sybachin[a], Karina A. Kisliak[a], Tatiana V. Dubinina[a]

[a] *Lomonosov Moscow State University, Department of Chemistry, 119991 Moscow, Russian Federation*

Effective photosensitizers with micromolar photodynamic activity *in vitro* were obtained based on water-soluble forms of hydrophobic substituted phthalocyanine complexes. To study the influence of heavy halogen atoms at the periphery of the macrocycle on the photochemical activity of phthalocyanines, bulky *para*-halo-phenoxy groups were introduced. Furthermore, *para*-*tert*-butyl-phenoxy and phenoxy groups were tested as peripheral substituents. The target phthalocyanines were found to be mixed type I/II photosensitizers capable of generating both singlet oxygen and superoxide anion radical. When going from *para*-chlorophenoxy to *para*-iodophenoxy substituents, an increase in the yield of singlet oxygen and a simultaneous decrease in the efficiency of superoxide anion radical generation were observed.

Water-soluble forms of hydrophobic aryloxy-substituted phthalocyanines were obtained as complexes with cyclodextrins. These solubilized forms demonstrated low cytotoxicity in the dark and high phototoxicity towards WI38, HCT166, MCF7, and A431 cell lines. The iodine-substituted complex exhibited the highest phototoxicity (IC_{50} = 7 μM).



We are grateful to the Russian Science Foundation No. 24-73-00062 for main support of this research.

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Structural characterisation of an on-surface reaction: Halogenated porphyrins on Cu(111)

Ailish Gray[a], Eleanor S. Frampton[b], Michael Clarke[a], Matthew Edmondson[a], Joseph Straw[a], Robert Templeton[b] and Alex Saywell[a]

[a] *University of Nottingham, School of Physics & Astronomy, University Park, Nottingham NG7 2RD, United Kingdom*
[b]*MAX IV Laboratory, Lund University, 22100 Lund, Sweden*

Surface-confined synthesis provides alternative reaction pathways to those utilised within solution-phase chemistry and offers a route to generating extended molecular architectures which may exhibit fascinating optical, magnetic, and electronic properties [1,2]. The novel reaction pathways by which on-surface synthesis proceeds are multistep processes, containing multiple reactive intermediates, and it can be non-trivial to characterise the underlying mechanisms. However, understanding such mechanisms is a vital prerequisite for controlling and optimising on-surface synthesis protocols.

The Ullmann-type coupling of halogenated molecules is well-studied by scanning probe microscopy (SPM) techniques under ultra-high vacuum (UHV) conditions. [3-4] We have previously utilised SPM in combination with x-ray photoelectron spectroscopy (XPS) to detail the reaction steps for brominated tetraphenyl porphyrin (BrxTPP) on the Cu(111) and Au(111) surfaces, and identified distinct reaction steps (including de-halogenation, metal organic framework formation, covalent coupling, and porphyrin metalation). [5] Here, we describe a complementary X-ray standing wave (XSW) study detailing the structural characterisation of BrxTPP on Cu(111). By employing XSW analysis, we obtain information on the adsorption geometry for specific chemical species within the various reaction steps, providing details on the mechanistic and structural evolution of an on-surface reaction.

REFERENCES

1. Auwärter, W. et al. Nat Chem 2015, 7 (2), 105.
2. Grill, L. et al. Nat. Chem. 2020, 12 (2), 115–130.
3. Shen et al., Nano Today, 2017, 13, 77–96.
4. Dong et al. Acc. Chem. Res., 2015, 48, 2765–2774.
5. Frampton, E. S. et al. ACS Appl. Nano Mater. 2025, 8 (24), 12608–12618.

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Extrinsic activation of an on-surface reaction

Ailish Gray[a], Eleanor S. Frampton[b], Michael Clarke[a], Matthew Edmondson[a], Jonathan Bradford[a], Liv Warwick[a], Nicholas Pearce[c], Neil R. Champness[c] and Alex Saywell[a]

[a] *University of Nottingham, School of Physics & Astronomy, University Park, Nottingham NG7 2RD, United Kingdom*
[b] *MAX IV Laboratory, Lund University, 22100 Lund, Sweden*
[c] *The University of Birmingham, School of Chemistry, B15 2TT Birmingham, U.K.*

On-surface synthesis (OSS) has become a well-established route to facilitate the coupling of molecular 'building blocks', giving rise to extended one- and two-dimensional molecular architectures. [1-3] Typically, such on-surface reactions are performed on a metallic surface, and the substrate often acts as both a support and a catalyst. However, the molecule-substrate hybridisation which occurs on metals can significantly alter the electronic structure of the molecular species and may inhibit the desired properties of the system (e.g. covalently coupled molecules acting as molecular wires or opto-electronic components within solid-state devices). One approach to ameliorating this issue is to utilise bulk insulator or insulating films, [4] but the corresponding reduction in substrate reactivity is likely to limit the available on-surface synthetic routes.

Here we study OSS utilising an extrinsic catalyst, i.e. a non-metallic substrate patterned with a reactive metal under ultra-high vacuum (UHV) conditions. Specifically, we build upon the wealth of work studying Ullmann-type reactions on metallic surfaces, by characterising the reactivity of a highly orientated pyrolytic graphite (HOPG) surface patterned with Au with respect to the covalent coupling of halogenated porphyrin species (Br_xTPP). Using a combination of low-temperature scanning tunnelling microscopy (LT-STM), temperature programmed X-ray photoelectron spectroscopy (TP-XPS) and near edge X-ray absorption fine structure (NEXAFS) measurements, we compare the progression of an on-surface reaction of Br_xTPP on Au/HOPG to our previous work on Cu and Au substrates. [5]

REFERENCES

1. Grill, L. & Hecht, S. Nat. Chem. 2020, 12, 115–130.
2. Clair, S. & de Oteyza, D. G. Chem. Rev. 2019, 119, 4717–4776.
3. Zhang, et al., Acc. Chem. Res. 2025, 58, 2179–2190.
4. Zhao, W. et al. Chem. Commun. 2016, 52 (90), 13225–13228.
5. Frampton, E. S. et al. ACS Appl. Nano Mater. 2025, 8 (24), 12608–12618.

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Porous structures based on cobalt corroles for the selective detection of carbon monoxide

Claude P. Gros[a], Laurie André,[a] Margerie Loze,[a] Ken Rapady,[a] Gaëlle Divoux,[a] Nicolas Desbois,[a] Stéphane Brandès,[a] Meddy Vanotti,[b] Virginie Blondeau-Patissier,[b]

[a] *Université Bourgogne Europe, ICMUB (UMR CNRS 6302), 9 av. Alain Savary, 21078 Dijon, France*
[b] *Institut FEMTO-ST (UMR CNRS 6174), 26 chemin de l'Epitaphe, 25030 Besançon, France*

Carbon monoxide (CO) is an odourless and colourless gas. Using selective and sensitive devices allowing CO detection at the *ppm* level is essential for the prevention of intoxication, which can lead to nausea, coma or even death. Corroles have shown to selectively bind CO *vs.* N_2, CO_2 and O_2. Supporting cobalt corroles with highly porous structures helps prevent their π-π stacking and thus ensures the targeted gas accessibility to the active cobalt sites. Our team has developed several porous materials integrating cobalt corroles which have been tested for CO and CO_2 co-detection: a corrole-based POP (Porous Organic Polymer) [1], some corrole-based COFs (Covalent Organic Frameworks) [2], a corrole-based Zr-MOF (Metal Organic Frameworks) and Zr-MOFs (PCN-222) hosting cobalt corroles withing their pores, by grafting to the zirconium cluster [3,4]. The synthesis, characterization, and gas sorption performances of these diverse materials will be presented. The specific surface area of the different materials was determined using the BET method and CO sorption measurements were recorded along with selectivity calculations against N_2, O_2 and CO_2.



Figure 1

REFERENCES

1. S. Brandès, V. Quesneau, O. Fonquernie, N. Desbois, V. Blondeau-Patissier, C. P. Gros, *Dalton Trans.*, **2019**, 48(31), p. 11651 11662.
2. J. Yang, L. André, N. Desbois, C. P. Gros, S. Brandès, *Mater. Today Chem.*, **2023**, 28, 101357.
3. M. Loze, S. Brandes, P. Fleurat-Lessard, N. Desbois, V. Blondeau-Patissier, C. P. Gros, L. André, *Chem. Eur. J.*, **2024**, 30, e202402148.
4. G. Divoux, M. Loze, Y. Rousselin, S. Brandès, C. P. Gros, N. Desbois, L. André, *Dalton Trans.*, **2025**, 54, 1784-1790.

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Virus-based adducts encapsulating corroles macrocycles to fight viral-infections

Claude P. Gros,[a] Shivani Kessavdjee-Djouma,[a,b] Nicolas Desbois,[a] Haziq Naseer Khan,[b] Tomas Moravec,[c] Nguyet-Thanh Ha Duong[b]

[a] *Université Bourgogne Europe, ICMUB (UMR CNRS 6302), 21000 Dijon, France*
[b] *Université Paris Cité, ITODYS (UMR CNRS 7086),75205 Paris Cedex 13, France*
[c] *Institute of Experimental Botany, Prague 6, 16502, Czech Republic*

Plant viruses are increasingly used in nanomedicine. Their capsids, composed of self-assembling protein subunits, are stable and have uniform shapes and sizes capable of encapsulating molecules (Fig.1). By genetically or chemically modifying capsid proteins, different functional groups can be added to their external and internal surfaces, allowing the grafting of molecules, especially drugs, to use these plant viruses as nanovectors. In this work, we focused on the development of nanovectors against monkeypox, an infectious disease caused by an orthopoxvirus (characterized by severe skin rashes). This viral infection has been declared a public health emergency of international concern by the WHO [1]. The announcement was made twice, once in May 2022 and again in August 2024. Since then, the disease has been under reinforced surveillance in France and Europe.
We have used the Tobacco Virus (TMV) as a nanovector for antiviral active compounds. TMV is a rod-shaped virus of 300 nm long and 18 nm in diameter. Its capsid allows a large number of therapeutic agents to be loaded inside its cavity, increasing their concentration and solubility. We have selected fluorinated corroles as antiviral agents, as some of which have shown very promising antiviral activity against the orthopoxvirus family [2]. These molecules can be encapsulated in the cavity of plant viruses in a high ratio, without affecting the structural integrity of the virus. Interestingly, the infection rate was reduced in the presence of encapsulated corroles compared to free corroles. Various corroles have also been synthesized for further covalent grafting onto the outer surface of TMV.

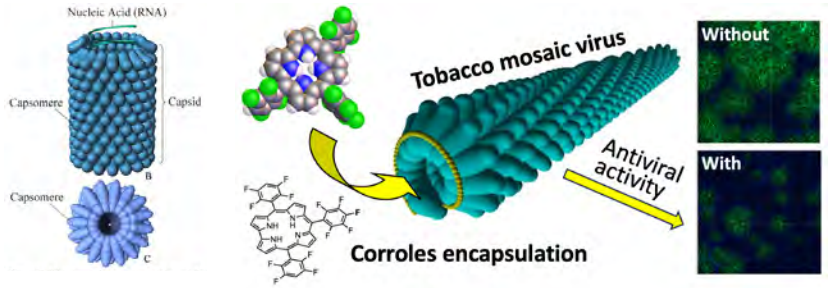


Figure 1

This work was supported by the ANRS Project COLORS (Contrat d'Initiation N°ANRS0652 - ECTZ292887).

REFERENCES

1. https://worldhealthorg.shinyapps.io/mpx_global/#3_Global_situation_update
2. S. Kappler-Gratias, et al., *ACS Infect. Dis.*, **2021**, 7, 2370–2382.
3. S. Kessavdjee-Djouma, T. Moravec, H. N. Khan, S. Kappler-Gratias, F. Gallardo, N. Desbois, N.-T.-H. Duong and C. P. Gros, Plant virus-corrole hybrids as bio-inspired antiviral nanomaterials, *ACS Infect. Dis.*, **2026**, submitted.

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Electronically Tuned Dipyrromethene and BODIPY Platforms for Selective Fluoride and Cyanide Detection

Huma[a] Harshita Saroj[a,b] Pankaj Arora[b] and Nitika Grover[a]

[a]*Department of Chemistry, BITS Pilani, Pilani Campus. Email: nitika.grover@pilani.bits-pilani.ac.in*
Birla Institute of Technology and Science, Pilani, Rajasthan-333031, India
[b]*Smart Materials and Sensing Devices (SMSD) Laboratory,*
Department of Electrical and Electronics Engineering,
Birla Institute of Technology and Science, Pilani, Rajasthan-333031, India

Molecular engineering of rapid, highly selective sensing platforms for hazardous ions remains an open challenge because of their very low environmental thresholds.[1-3] Hence, there is an urgent need for robust, efficient molecular systems that enable sensitive ion recognition in both solvent and solid states. To address this, we have developed two molecular scaffolds selective for either fluoride or cyanide detection. First, we designed a series of meso-aryl 1,9-bisbenzothiazole-substituted dipyrromethenes (DPMEs) as a fluoride-responsive system. Next, we converted DPMEs into their corresponding BODIPY derivatives to generate a cyanide-trapping platform. To explore the influence of electronic effects on sensing behavior, various electron-donating and electron-withdrawing substituents were introduced at the meso-aryl position of the benzothiazole-substituted DPME core. Interestingly, the 5-pentafluorophenyl-1,9-bisbenzothiazole DPME exhibited the highest selectivity toward fluoride ions, accompanied by a distinct color change from pink to blue. The sensing mechanism was further studied via absorption and fluorescence spectroscopy, which revealed a significant red shift upon addition of the F^- ion. Notably, this sensing process with the DPME derivative was fully reversible. NMR titrations confirmed that the pronounced optical response originates from strong interactions of fluoride with the pyrrolic N–H site. In BODIPY systems, the sensing preference shifted from fluoride to cyanide. In these BODIPY frameworks, nucleophilic attack of cyanide at the meso-position disrupts π-conjugation, leading to rapid fluorescence quenching. To extend practical applicability, the most responsive chromophores were integrated into an SPR device to construct solid-state sensing platforms. Overall, the robust and well-defined spectral responses highlight the promise of this tunable dipyrromethene/BODIPY system for environmental monitoring and safety-critical detection of fluoride and cyanide ions.

REFERENCES

1. P. A. Gale, C. Caltagirone, *Chem. Soc. Rev*. **2015**, *44*, 4212–4227.
2. D. Beer, P. A. Gale, *Angew. Chem. Int. Ed.* **2001**, *40*, 486–516.
3. P. A. Gale, J. T. Davis, R. Quesada, *Chem. Soc. Rev.* **2017**, *46*, 2497–2519.

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Versatile Nitration of BODIPY Dyes Using NO_2BF_4: Effects of Nitro Substituents on Spectroscopic and Self-Assembly Properties

Caroline Gwaro[a,d] Caroline Ndung'U,[a,d] Petia Bobadova-Parvanova,[b] Dylan Goliber,[b] Quynh Do,[a] Ashley R. Walker,[a] Evan Murders,[a] Daniel LaMaster,[c] Frank R. Fronczek,[a] Jayne Garno,[a] and Maria da Graça H. Vicente[a,*]

[a]*Department of Chemistry, Louisiana State University, Baton Rouge, 70803 LA*
[b]*Department of Chemistry and Fermentation Sciences, Appalachian State University, Boone, NC 28608*
[c]*Department of Chemistry, Talladega College, Talladega, AL 35160*
[d]*C.G. and C.N. contributed equally.*

Nitro-substituted BODIPYs are important precursors in organic synthesis, as nitro groups can be reduced to amines and other functionalities, which can be further derivatized [1]. In addition, the strong electron-withdrawing character of nitro groups modulates the electronic and optical properties of BODIPYs, allowing for the development of promising derivatives for applications in bio-imaging, PDT, and polarity sensing [2, 3]. However, nitration of BODIPY dyes remains underexplored, as conventional methods employ harsh reaction conditions and yield the nitrated BODIPYs in low yields [3]. Therefore, there's a need to explore other methods for nitrating BODIPYs with high yields and under mild reaction conditions. This presentation explores nitration of BODIPY dyes using nitronium tetrafluoroborate (NO_2BF_4). Our study has shown that NO_2BF_4 regioselctively nitrates BODIPY dyes in high yields and under mild reaction conditions. The synthesis, self-assembly, experimental, and computational photophysical properties of the nitrated chromophores will be presented.

REFERENCES

1. Esnal, I.; Bañuelos, J.; López Arbeloa, I.; Costela, A.; Garcia-Moreno, I.; Garzón, M.; Agarrabeitia, A. R.; José Ortiz, M. Nitro and Amino BODIPYS: Crucial Substituents to Modulate Their Photonic Behavior. RSC Adv. 2013, 3 (5), 1547–1556. https://doi.org/10.1039/C2RA22916A.
2. Gwaro, C.; Ndung'U, C.; Bobadova-Parvanova, P.; Goliber, D.; Do, Q.; Walker, A. R.; Murders, E.; LaMaster, D.; Fronczek, F. R.; Garno, J.; Vicente, M. da G. H. Effects of Nitro-Substitution on the Spectroscopic and Self-Assembly Properties of BODIPY Dyes. ACS Omega 2025, 10 (15), 14723–14737. https://doi.org/10.1021/acsomega.4c08799.
3. Zarcone, S. R.; Yarbrough, H. J.; Neal, M. J.; Kelly, J. C.; Kaczynski, K. L.; Bloomfield, A. J.; Bowers, G. M.; Montgomery, T. D.; Chase, D. T. Synthesis and Photophysical Properties of Nitrated Aza-BODIPYs. New J. Chem. 2022, 46 (9), 4483–4496. https://doi.org/10.1039/D1NJ05976A.

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On-Surface Synthesis of π-Extended Subphthalocyanine-Based Systems

Marta Gómez-Gómez,[a] **Jorge Lobo-Checa,**[b,c] **Jorge Labella,**[d] **Tomás Torres**[a,e,f]

[a]*Organic Chemistry Department, Universidad Autónoma de Madrid, 28049, Madrid, Spain*
[b]*Instituto de Nanociencia y Materiales de Aragón, CSIC-Universidad de Zaragoza, 50009, Zaragoza, Spain*
[c]*Departamento de Física de la Materia Condensada, Universidad de Zaragoza, 50009, Zaragoza, Spain*
[d]*Department of Molecular Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan*
[e]*IMDEA-Nanociencia, c/Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain*
[f]*Institute for Advanced Research in Chemical Sciences, Campus de Cantoblanco, 28049 Madrid, Spain*

In past decades, on-surface synthesis (OSS) has emerged as a powerful tool to prepare 2D materials from simple building blocks bearing reactive groups (e.g., halogen atoms).[1] If these building blocks present a bowl-shaped –rather than flat– structure, the peripheral (reactive) groups would be oriented toward the surface when a bowl-down configuration is adopted (Figure 1).[2,3] This orientation is expected to influence the electronic and structural properties of such substituents. Based on this premise, several open questions arise: does the regiochemistry on the coupling affect the properties of the generated material? Could the bowl shape affect to the on-surface behavior of organic molecules, potentially generating new unexpected structures?

Here, it is demonstrated that the bowl-shaped subphthalocyanines (SubPcs) serve as excellent starting materials for the "toposelective" preparation of 0D, 1D and 2D curved π-systems (Figure 1). Remarkably, the regiochemistry is observed to influence both the order control during polymerization and the electronic properties of the resulting 2D material, leading to π-extended, porous, and chiral polymers with enhanced electronic delocalization. Going one step further, the size, shape, and even chemical nature (covalent or metalorganic) of the resulting product depend on the halogen used in the on-surface Ullmann coupling, showing distinct behaviors for bromine, chlorine, and fluorine.

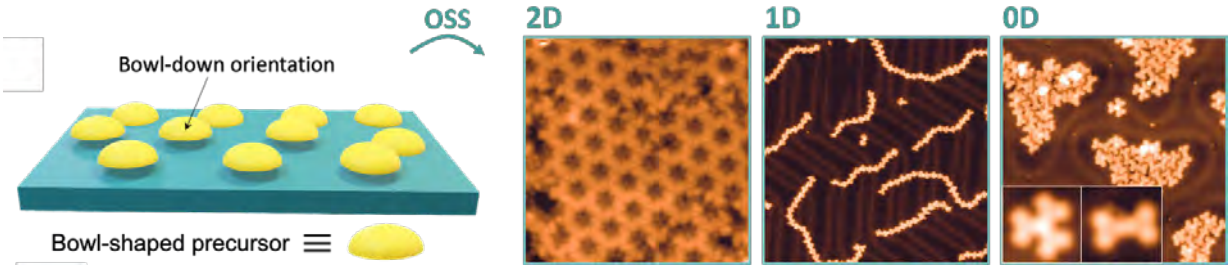


Figure 1. On-surface synthesis of 0D, 1D and 2D curved π-systems.

REFERENCES

1. Clair, S; de Oteyza D.G. *Chem. Rev.* **2019**, *119*, 4717–4776.
2. Lavarda, G; Labella, J; Martínez-Díaz, M. V.; Rodríguez-Morgade, M. S.; Osuka, A. Torres, T. *Chem. Soc. Rev.* **2022**, *51*, 9482–9619.
3. Labella, J.; Lavarda, G.; Hernández-López, L.; Aguilar-Galindo, F.; Díaz-Tendero, S.; Lobo-Checa, J.; Torres, T. *J. Am. Chem. Soc*. **2022**, *144*, 16579–16587.

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Bowl-to-Bowl Inversion in Subphthalocyanines: S_N2 vs. S_N1 Pathways at a Tetracoordinate Boron

Marta Gómez-Gómez,[a] Jorge Labella,[b] Tomás Torres[a,c,d]

[a]*Organic Chemistry Department, Universidad Autónoma de Madrid, 28049, Madrid, Spain*
[b]*Department of Molecular Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan*
[c]*IMDEA-Nanociencia, c/Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain*
[d]*Institute for Advanced Research in Chemical Sciences, Campus de Cantoblanco, 28049 Madrid, Spain*

Bowl-to-bowl (BtB) inversion is an emblematic dynamic process of non-planar π-systems.[1] Unlike corannulenes and sumanenes, the presence of an axial ligand in subphthalocyanines (SubPcs) sterically locks their BtB inversion.[2] However, it becomes feasible upon removal of the axial ligand, yielding a borenium cation. In this context, the configurational evolution of stereocenters has long served to uncover the factors governing such processes, establishing guidelines to distinguish between S_N1 and S_N2 mechanisms.[3] In boron chemistry, however, the stereochemical outcome of reactions at tetrahedral boron centers remains poorly understood, as the isolation of stable, enantiopure boron species for precise configurational tracking remains far from trivial.

Herein, enantiopure SubPcs are employed as stereochemical probes to unravel the BtB inversion in boron-containing compounds. Thus, we conduct an in-depth study of the SubPcs axial ligand exchange, integrating both experimental and theoretical approaches. Our results suggest that the reaction primarily proceeds via a bimolecular σ-bond metathesis mechanism (Figure 1), which predominantly leads to retention of configuration. However, partial inversion of the configuration may occur through a S_N1-like mechanism, in which a pseudo-planar SubPc transition state is reached (Figure 1). Strikingly, the extent of inversion is modulated by multiple factors: the nature of the reagents, the electronic properties of the SubPc core, its substitution pattern, and the axial leaving group. Together, these findings offer fundamental insight not only into the long-overlooked stereochemical course of boron-centered substitution reactions, but also into the configurational dynamics of bowl-shaped π-systems.

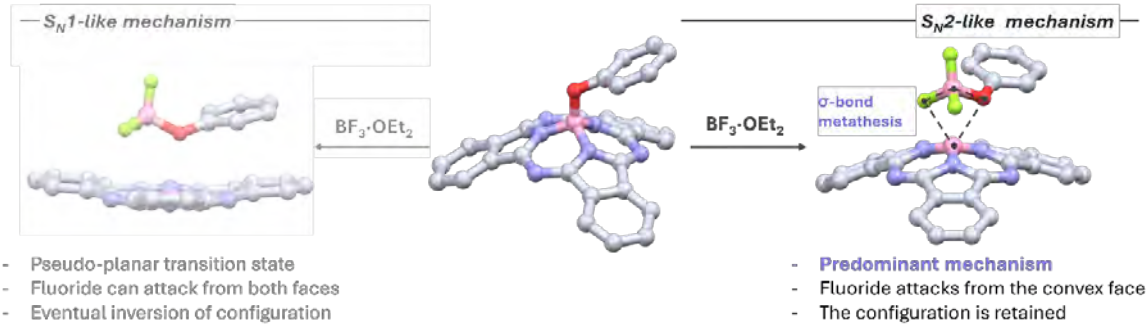


Figure 1. Mechanisms involved in the axial ligand exchange reaction between phenol- and fluorine-SubPcs.

REFERENCES

1. Saito, M.; Shinokubo, H; S. Hidehiro. *Mater. Chem. Front.* **2018**, *2*, 635–661.
2. Gómez-Gómez, M.; Laforga-Martín, J.; Labrador-Santiago, J.; Labella, J.; Torres T. *ChemistryEurope* **2025**, DOI: 10.1002/ceur.202500244.
3. F. A. Carey, R. J. Sundberg. Advanced Organic Chemistry: Part A: Structure and Mechanisms. Springer-Verlag New York Inc., **2008**.

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The high diversity of oxygen reactivity in bacterial terminal oxidases

Raaif Siddeeque[a], Lucia Heger[b], Thorsten Friedrich[b], Frédéric Melin[a] and Petra Hellwig[a*]

[a] *Laboratoire de Bioélectrochimie et Spectroscopie, UMR 7140, Chimie de la Matière Complexe, Université de Strasbourg – CNRS 4, rue Blaise Pascal, 67081 Strasbourg, France * hellwig@unistra.fr*
[b] *Institut für Biochemie, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany;*

Terminal oxidases are critical for aerobic respiratory chains of prokaryotes and eukaryotes, responsible for the final step in the electron transport chain. These membrane proteins catalyse the transfer of electrons from reduced electron carriers (such as cytochrome c or quinols) to the terminal electron acceptor, molecular oxygen, thereby reducing it to water. They play a pivotal role in aerobic respiration and energy metabolism, adapting to diverse environmental and physiological needs across different organisms. [1,2]
First an overview of the electrochemical properties of terminal oxidases from different organisms will be given and their high degree of adaptivity with redox potentials spanning more than 500 mV discussed, with a special focus on bacterial oxidases. The electrocatalytic response observed by means protein film voltammetry will be described, giving insight into the rich and complex electron and proton transfer catalysed by these essential enzymes.
The superfamily of cytochrome bd oxidases are solely present in prokaryotes. These enzymes play a crucial role in protection against oxidative stress, in virulence, adaptability and antibiotics resistance.[3,4] Recent structural data, electrochemical and spectroscopic studies allowed obtaining information on the oxygen reduction, coupled protonation processes, and the interaction with small molecules that rule the signaling processes in the biological cell, including NO.

REFERENCES

1. Melin, F., Hellwig, P. ‘Redox Properties of the Membrane Proteins from the Respiratory Chain' (2020), Chem. Rev., 120, 10244–10297.
2. Hellwig, P. 'The electrochemical properties of the highly diverse terminal oxidases from different organisms' (2025) Bioelectrochemistry 165, 108946.
3. Borisov, V.B. Siletsky, S.A. Paiardini, A. Hoogewijs, D. Forte, E. Giuffrè, A. Poole, R.K. ‘Bacterial Oxidases of the Cytochrome bd Family: Redox Enzymes of Unique Structure, Function, and Utility As Drug Targets’ (2020) Antioxid. Redox Signal. 34, 16, 1280-1318.
4. Safarian, S.; Hahn, A.; Mills, D.J.; Radloff, M.; Eisinger, M.L.; Nikolaev, A.; Meier-Credo, J.; Melin, F.; Miyoshi, H., Gennis, R.B.; Sakamoto, J.; Langer, J.D.; Hellwig, P.; Kühlbrandt, W.; Michel, H. ‘Active site rearrangement and structural divergence in prokaryotic respiratory oxidases’ (2019), Science, 366, 100-104.

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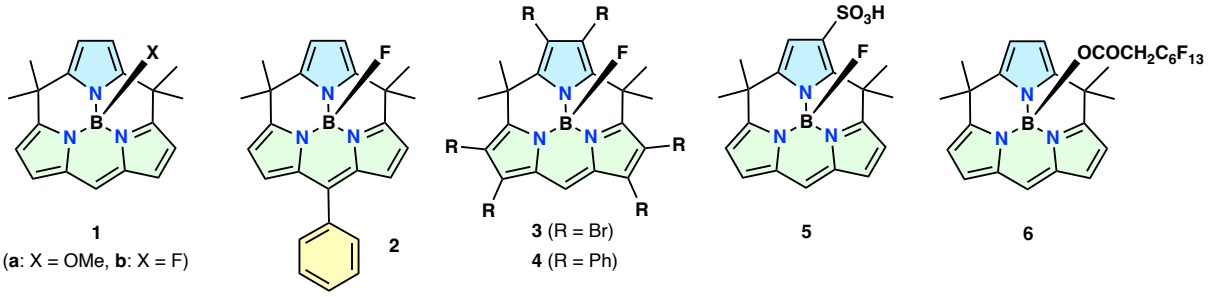
Peripheral and axial functionalization of superacid-resistant macrocyclic BODIPYs

Gentaro Honda[a], **Keita Watanabe**[a], **Yuki Ide**[b], **Yasuhide Inokuma**[a,b]

[a]*Division of Applied Chemistry, Faculty of Engineering, Hokkaido University, Japan*
[b]*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University*

Based on our discovery of a synergistic boron chelation effect in calix[3]pyrrole, we recently developed superacid-resistant macrocyclic boron–dipyrromethenes (BODIPYs) that retain bright fluorescence even in non-diluted superacids without deboronation. [1],[2] To modulate the absorption and emission wavelengths as well as solubility in various media, we examined the peripheral and axial functionalization of macrocyclic BODIPY **1**.

While BODIPY **1a** was obtained in 46% yield through the condensation reaction between boron–tripyrrane and triethyl orthoformate, an analogous reaction using benzoyl chloride and BF_3•OEt_2 afforded *meso*-phenyl derivative **2**. Owing to the π-conjugative interactions of the phenyl group, **2** exhibited red-shifted fluorescence reaching 700 nm compared to **1b**. Treatment of **1b** with an excess amount of bromine quantitatively yielded hexabromo analogue **3**. Suzuki–Miyaura cross coupling reaction of **3** with phenylboronic acid furnished hexaphenyl derivative **4** in 4% yield. BODIPY **4** also exhibited red-shifted fluorescence at 537 and 591 nm in concentrated sulfuric acid. Aromatic electrophilic substitution of **1b** with chlorosulfonic acid proceeded at the isolated pyrrole moiety to give sulfonylated analogue **5** which showed improved solubility in water. Boron-axial ligand exchange of **1a** with tridecafluorooctanoic acid furnished fluorous-tagged analogue **6** in 86% yield. Compound **6** was soluble in fluorous solvents; for example, its solubility in perfluoromethylcyclohexane was 49 mg/L. Compound **6** was used as a turn-on type fluorescent indicator for perfluorooctanoic acid in fluorous media. In this presentation, we will disclose the detailed synthetic procedures and photophysical properties of peripherally and axially functionalized superacid-resistant macrocyclic BODIPYs.



1 (**a**: X = OMe, **b**: X = F) **2** **3** (R = Br) **4** (R = Ph) **5** **6**

REFERENCES

1. Y. Inaba, Y. Nomata, Y. Ide, J. Pirillo, Y. Hijikata, T. Yoneda, A. Osuka, J. L. Sessler, Y. Inokuma, *J. Am. Chem. Soc.* **2021**, *143*, 12355.
2. K. Watanabe, G. Honda, Y. Inaba, T. Nakajima, J. P. Gong, Y. Ide, M. Gao, T. Yoneda, Y. Inokuma, *Nat. Commun.* in revision.

POSTERS

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Hydrogen Atom Abstraction by μ-Oxo Iron Porphyrin Dimers in Dioxygen-Promoted Catalytic Deformylation of Aldehydes

Kai-Chun, Hsu[a,b,c], Bhakyaraj Kasia[a,d,e], Tanmoy Pain[a], Chen-Hsiung Hung[a]

[a] *Institute of Chemistry, Academia Sinica, Nankang, Taipei 115201, Taiwan.*
[b] *Nano Science and Technology Program, Taiwan International Graduate Program, Academia Sinica, Taipei 115201, Taiwan*
[c] *Department of Chemistry, National Taiwan University, Taipei 106319, Taiwan*
[d] *Molecular Science and Technology Program, Taiwan International Graduate Program, Academia Sinica, Taipei 115201, Taiwan*
[e] *Department of Chemistry, National Tsing Hua University, Hsinchu 300044, Taiwan*

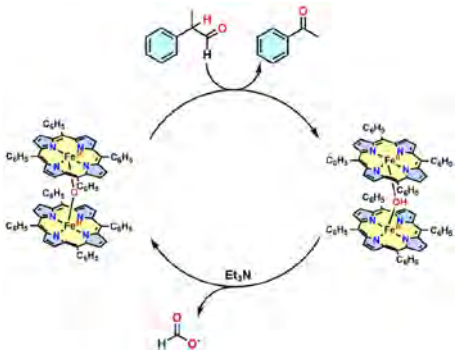
POSTERS

Iron porphyrins play essential roles in biological oxidation and have been widely studied as biomimetic catalysts. Among them, μ-oxo iron(III) porphyrin dimers are commonly observed intermediates in oxidative processes, yet their direct involvement in hydrogen atom abstraction (HAA) reactions remains insufficiently explored.

Herein, we report a catalytic deformylation reaction of aldehydes promoted by dioxygen using a μ-oxo iron porphyrin dimer, $[Fe(TPP)]_2O$ (TPP = tetraphenylporphyrin), as the catalyst. Using 2-phenylpropanal (2-PPA) as a model substrate, efficient conversion to acetophenone was observed under aerobic conditions. Mechanistic studies indicate that the reaction proceeds via initial hydrogen-atom abstraction from the aldehyde by the μ-oxo iron species, generating a carbon-centered radical intermediate. The formation of radical intermediates was confirmed by EPR spin-trapping experiments, while kinetic analysis provided further evidence supporting the HAA step. The catalytic system exhibits high efficiency, with yields up to 97% under optimized conditions.

These results provide direct experimental evidence that μ-oxo iron porphyrin dimers can function as active hydrogen atom abstractors in oxidative catalysis. This work highlights the potential role of μ-oxo iron porphyrins in biomimetic oxidation chemistry and contributes to a better understanding of iron porphyrin-mediated radical transformations. Ongoing work in our group explores related porphyrin systems for proton-coupled electron transfer (PCET) processes in electrocatalytic nitrate reduction.

This work was recently published in Dalton Transactions (2026).



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ROS-Regulating Hydrogel-Based Platform Coating to Enhance Stem Cell Function

Kim Hyun Woo[a,b], Kun Na[a,b]*

[a] *The Catholic University of Korea Department of Biotechnology The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Bucheon-si, Gyeonggi-do 14662, Republic of Korea*
[b] *The Catholic University of Korea Department of Biomedical-Chemical Engineering The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Bucheon-si, Gyeonggi-do 14662, Republic of Korea*
** Corresponding author at: Department of BioMedical-Chemical Engineering, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Bucheon-si, Gyeonggi-do 14662, Republic of Korea * kna6997@catholic.ac.kr*

Stem cells have emerged as promising therapeutics in regenerative medicine due to their self-renewal capacity and paracrine signaling, including exosome and growth factor secretion [1]. However, stem cell–based therapies have limitations, including immune rejection, manufacturing scalability constraints, and incomplete or inconsistent differentiation [2]. Overcoming these challenges is essential for achieving safe, reproducible, and clinically effective translation.

Based on previous studies showing that optimal levels of ROS facilitate stem cell activation, we developed a cell-supportive platform with Reactive oxygen species (ROS) triggered activation of stem cells. Here, we fabricated a physically stable and coatable hydrogel platform, termed ‘PG-PP’, by mixing a polymer-photosensitizer conjugate (PP), which generates reactive oxygen species (ROS), into a polyphenol-gelatin (PG) network. The actual physicochemical stability of the PG-PP platform was demonstrated through evaluations of its rheological behavior and compressive stability. Multiple assays were performed to confirm the stem cell activation induced by the optimal ROS release from the PG-PP platform. Using adipose-derived stem cells (ADSCs) in vitro, cell proliferation was significantly enhanced by about 198% at 72 h compared with conventional culture plates and other controls. Additionally, active cell division was induced by a reduction in the G0/G1 phase population, accompanied by confirmed downregulation of senescence-related markers p16 and p21. Furthermore, Optimal ROS release from the platform demonstrated that the PG-PP platform significantly enhanced exosome and paracrine factor secretion, as well as chondrogenic and adipogenic differentiation staining, compared to the control group.

Overall, the PG-PP platform provides mechanically stable, biofunctional support, thereby enhancing stem cell activity. This strategy represents a scalable and promising approach for advancing next-generation cell-based therapeutics

REFERENCES

1. Song, Na, Martijn Scholtemeijer, and Khalid Shah. "Mesenchymal stem cell immunomodulation: mechanisms and therapeutic potential." Trends in pharmacological sciences 41.9 (2020): 653-664.
2. Hoang, Duc M., et al. "Stem cell-based therapy for human diseases." Signal transduction and targeted therapy 7.1 (2022): 272.

POSTERS

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Enhancing Charge-Separated State Persistence via *N*-Linked Zinc Phthalocyanine-Pyrroloperylenediimide (ZnPc-*N*-PDI) Donor–Acceptor Architecture

Chamari V. Ileperuma[a], Jose Garcés-Garcés[b], Ana M. Gutiérrez-Vílchez[b], Ángela Sastre-Santos[b], Fernando Fernández Lázaro*[b], Francis D'Souza*[a]

[a]*Department of Chemistry, University of North Texas at Denton, 1155 Union Circle, #305070, Denton, TX 76203-5017 (USA)*
[b]*Área de Química Orgánica, Instituto de Bioingeniería, Universidad Miguel Hernández, Avda. de la Universidad s/n 03203 Elche (Spain)*

One of the key strategies in developing artificial photosynthesis, organic photovoltaics (OPVs), and photo-driven charge-separation platforms is designing π-conjugated donor–acceptor (D–A) molecular systems. Effective energy conversion needs both long-lived charge-separated (CS) states and rapid photoinduced charge separation, which have been enabled mainly by covalently linked D–A dyads [1-3]. A zinc phthalocyanine-pyrroloperylenediimide dyad connected through a nitrogen heteroatom (PDI-*N*-ZnPc) has been newly synthesized and characterized. Solvent polarity-dependent singlet-singlet energy transfer and electron transfer quenching were observed from absorption and steady-state fluorescence studies. Electrochemical and spectroelectrochemical analyses enabled the assessment of the redox potentials of the donor and acceptor moieties, as well as the spectral characterization of their one-electron oxidation and reduction products. DFT studies were conducted to examine the geometry and electronic structure, as well as how *N*-connectivity influences the relative orientation of the entities. Furthermore, time-dependent DFT studies helped establish the different excited states responsible for charge separation. An energy diagram was then created to visualize various photophysical events. Finally, femtosecond transient absorption spectral studies were performed in both nonpolar and polar solvents to observe energy and electron transfer processes. The kinetic data were analyzed using both global and target analyses. The key findings of this study were the prolonged persistence of the charge-separated state in this dyad, compared with previously reported ZnPc-PDI dyads with carbon-carbon connectivity [3], highlighting the importance of heteroatom linkage in regulating electron-transfer dynamics in donor-acceptor conjugates.

REFERENCES

1. C. V. Ileperuma, J. Garcés-Garcés, A. M. Gutiérrez-Vílchez, Á. Sastre-Santos, F. Fernández-Lázaro, F. D'Souza, *ChemPhotoChem* **2025**, *0*, e202500238.
2. B. Sekaran, A. Dawson, Y. Jang, K. V. MohanSingh, R. Misra, F. D'Souza, *Chem. Eur. J.* **2021**, *27*, 14335-14344.
3. N. Zink-Lorre, E. Font-Sanchis, S. Seetharaman, P. A. Karr, Á. Sastre-Santos, F. D'Souza, F. Fernández-Lázaro, *Chem. Eur. J.* **2019**, *25*, 10123-10132.

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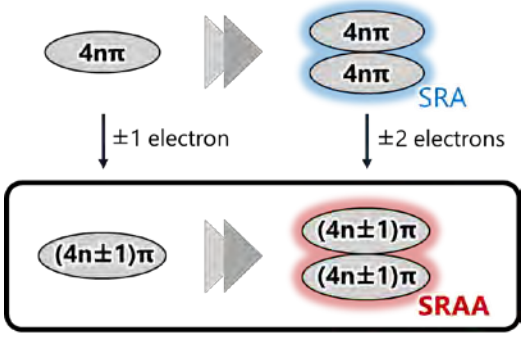
Stacked-Ring Antiaromaticity: Experimental Evidence and Structure–Property Relationships in Stacked Dimers of Cyclic Conjugated Radicals

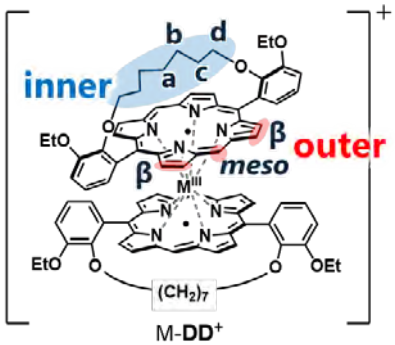
Wataru Imanaka[a], Satoshi Toyama[a], Shohei Saito[a], Ken-ichi Yamashita[a,b]

[a]*Department of Chemistry, Graduate School of Science, The University of Osaka*
[b]*Innovative Catalysis Science Division, Institute for Open and Transdisciplinary Research Initiatives (ICS-OTRI), The University of Osaka*

Aromaticity is one of the most fundamental chemical concepts for understanding the properties of cyclic π-conjugated compounds. While classical aromaticity is defined for a single cyclic π-conjugated system, the concept has been extended to stacked dimers of π-conjugated systems. Stacked-Ring Aromaticity (SRA), which refers to the aromatic character exhibited by stacked dimers of 4nπ conjugated rings, was theoretically proposed in 2007[1] and experimentally demonstrated in 2019.[2] Here, we further extend this concept and propose Stacked-Ring Antiaromaticity (SRAA), which is predicted to emerge in stacked dimers of (4n ± 1)π cyclic conjugated radicals on the basis of the π-electron counting rules for aromatic and antiaromatic systems. Focusing on oxidized cationic forms of rare-earth porphyrin double-decker complexes, we designed a series of new complexes, M-**DD**$^+$ (M = Lu, Y, and La), bearing alkylene straps above the porphyrin rings to enable a detailed evaluation of magnetic shielding effects arising from antiaromaticity using ^{1}H NMR spectroscopy.

For Lu-**DD**$^+$ and Y-**DD**$^+$, the inner alkylene protons appeared within the typical chemical shift range of ordinary methylene protons, suggesting that the complexes exhibit only weak SRAA. In contrast, La-**DD**$^+$ displayed pronounced downfield shifts of the inner alkylene protons and an upfield shift of the outer *meso* protons, indicating an enhanced paratropic ring current contribution. We will discuss structure–property relationships underlying these observations along with the results of quantum chemical calculations.





REFERENCES

1. Corminboeuf, C.; Schleyer, P. v. R.; and Warner, P. *Org. Lett.* **2007**, *9*, 3263−3266.
2. Nozawa, R.; Kim, J.; Oh, J.; Lamping, A.; Wang, Y.; Shimizu, S.; Hisaki, I.; Kowalczyk, T.; Fliegl, H.; Kim, D.; Shinokubo, H. *Nat. Commun.* **2019**, *10*, 3576−3582.

POSTERS

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Adamantane *vs* cyclohexane: how the bulkiness of phthalocyanines' substituents affects their properties

Umit Isci[a], Zeynel Şahin[a], Filippo Monti[b], Daniele Veclani[b], Barbara Ventura[b], Fabienne Dumoulin[c]

[a] *Marmara University, Faculty of Technology, Department of Metallurgical and Materials Engineering, Maltepe, Istanbul, Türkiye*
[b] *Istituto per la Sintesi Organica e la Fotoreattività (ISOF), Consiglio Nazionale delle Ricerche (CNR), Via Piero Gobetti 101, Bologna, 40129 Italy*
[c] *Acıbadem Mehmet Ali Aydinlar University, Graduate School of Natural and Applied Sciences, Ataşehir, 34752 Istanbul, Türkiye*

The substitution pattern of phthalocyanines is usually thought in terms of the number and position of substituents, as well as the chemical function that attaches the substituents to the phthalocyanine macrocycle. Those can indeed have huge effects [1-2]. Very frequently, the alkyl type of the substituent itself is less considered, even though its bulkiness can actually have tremendous effects [3].
In this work, we investigated how adamantyl moieties, among the bulkier alkyl moieties, affect the behavior of phthalocyanines compared to smaller cyclohexyl substituents through combined experimental and theoretical investigations.

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REFERENCES

1. Kobayashi, N.; Ogata, H.; Nonaka, N.; Luk'yanets, E. A., Effect of peripheral substitution on the electronic absorption and fluorescence spectra of metal-free and zinc phthalocyanines. *Chem. Eur. J.* **2003,** *9* (20), 5123-34.
2. Topal, S. Z.; İşci, Ü.; Kumru, U.; Atilla, D.; Gürek, A. G.; Hirel, C.; Durmuş, M.; Tommasino, J.-B.; Luneau, D.; Berber, S.; Dumoulin, F.; Ahsen, V., Modulation of the electronic and spectroscopic properties of Zn(II) phthalocyanines by their substitution pattern. *Dalton Trans.* **2014**, *43(18)*, 6897-6908.
3. Zorlu, Y.; Kumru, U.; İşci, Ü.; Divrik, B.; Jeanneau, E.; Albrieux, F.; Dede, Y.; Ahsen, V.; Dumoulin, F., 1,4,8,11,15,18,22,25-Alkylsulfanyl phthalocyanines: effect of macrocycle distortion on spectroscopic and packing properties. *Chemical Commun.* **2015,** *51* (30), 6580-6583.

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Water-soluble, thiolate-ligated Zn/Fe porphyrins

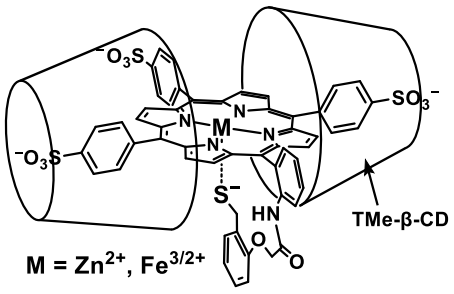
Yuto Isoda[a], Atsuki Nakagami[a], Qiyue Mao[a], Masahito Kodera[a], Hiroaki Kitagishi[a]

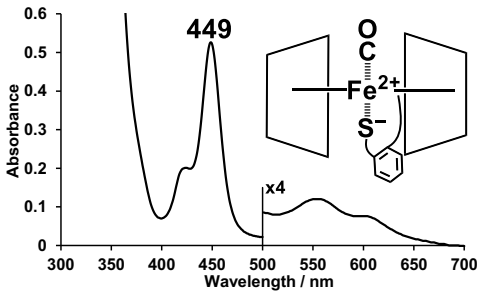
[a]*Faculty of Science and Engineering, Doshisha University*

Cytochrome P450 (P450) is a monooxygenase enzymes that share a conserved fold in which the heme iron is axially ligated by a thiolate ligand. Various synthetic thiolate-ligated metalloporphyrins have been proposed as well-defined models to probe the influence of this strongly electron-donating ligand on the distinctive spectroscopic signatures and catalytic behaviors of P450. However, there is no synthetic P450 model that retains its thiolate ligation in aqueous media due to the chemical instability of the thiolate.

So far, our group has constructed neutral N-ligated heme models that function in water, through host-guest inclusion complexation of iron tetrakis(4-sulfonatophenyl)porphyrin with methylated cyclodextrins (TMe-β-CDs) [1]. In this study, we report the first thiolate-ligated heme model that remains stable in aqueous solution at room temperature. We synthesized SAc-MTPPS, which incorporates a ligand arm directed toward the metal center, inspired by a previous SR model complex [2]. Then, we prepared the 1:2 inclusion complex with TMe-β-CD in aqueous solution to afford SAc-MTPPS/TMe-β-CD. In this complex, TMe-β-CD is expected to provide steric shielding around the porphyrin, thereby suppressing porphyrin aggregation and suppressing oxidative decomposition of the thiolate.

Spectroscopic characterization of SAc-MTPPS/TMe-β-CD was performed in 0.2 M NaOH aqueous solution, where base-promoted deacetylation generated the corresponding thiolate-ligated structure ([S$^-$−M]) (Figure 1). To assess thiolate coordination, the redox-inactive Zn porphyrin analogue was first examined. The UV-vis and NMR spectral changes observed for SAc-ZnTPPS/TMe-β-CD provided clear evidence for the formation of [S$^-$−Zn] complex. Next, as spectroscopic features of carbon monoxide (CO) adducts of P450 are widely used as a criterion of [S$^-$−Fe], we prepared the CO-bound form of SAc-FeTPPS/TMe-β-CD ([S$^-$−Fe^{2+}−CO]). The UV-vis spectrum of [S$^-$−Fe^{2+}−CO] exhibited a Soret absorption maximum at around 450 nm, which is clearly consistent with native P450 (Figure 2). In addition, resonance Raman spectroscopy combined with isotope-shift analysis enabled assignment of the ν_{Fe-CO} (461 cm^{-1}) and ν_{C-O} (1961, 1989 cm^{-1}) stretching frequencies. These frequencies are assigned to the established correlation line for thiolate-ligated hemes in the ν_{Fe-CO}/ν_{C-O} plot [3].





REFERENCES

1. Kitagishi, H.; Kano, K. *Chem. Commun.* **2021**, *57*, 148–173.
2. Higuchi, T.; Uzu, S.; Hirobe, M. *J. Am. Chem. Soc.* **1990**, *112* (19), 7051–7053.
3. Spiro, T.; Wasbotten, I. *J. Inorg. Biochem.* **2005**, *99* (1), 34–44.

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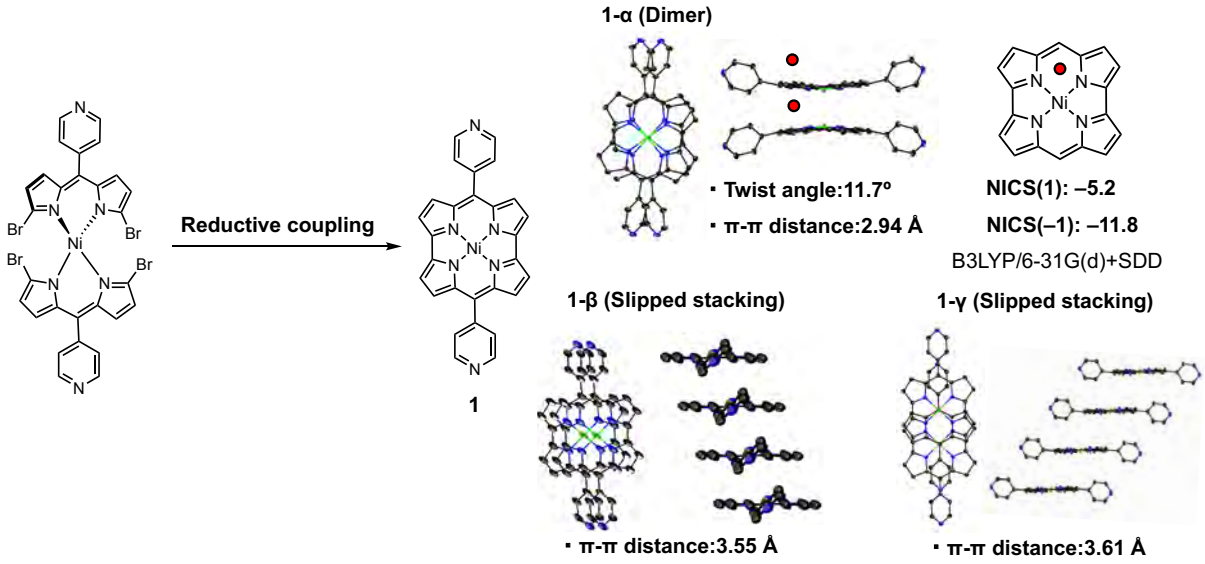


Synthesis, crystal polymorphism, and methylation of Ni(II) dipyridylnorcorrole

Koshiro Isono[a], **Shiori Itabuchi**[a], **Hideaki Takano**[a], **Hiroshi Shinokubo**[a]

[a]*Department of Molecular and Macromolecular Chemistry, Graduate School of Engineering, Nagoya University, Chikusa-ku, Nagoya464-8603, Japan*

Ni(II) norcorroles with various *meso*-substituents have been synthesized. Ni(II) pentafluorophenylnorcorrole exhibits stacked-ring aromaticity.[1] Trialkoxyphenyl-substituted Ni(II) norcorroles form meso phases.[2] Herein, we disclose the synthesis and structures of Ni(II) dipyridylnorcorrole **1**. Norcorrole **1** afforded three crystal polymorphs from different solvents used for crystallization. In particular, **1** forms a closely stacked dimer with a twist angle of 11.2° and a π–π stacking distance of 2.94 Å in crystal **1-α**. The NICS(1) and NICS(–1) values of **1-α** were –5.2 and –11.8 ppm, respectively, indicating the emergence of stacked-ring aromaticity. Crystals **1-β** and **1-γ** exhibit infinite one-dimensional stacking arrays with a slipped π-stacking arrangement with the interplanar distances of 3.55 and 3.61 Å, respectively. NMR titration experiments revealed that **1** forms a dimer in solution. In addition, *N*-methylation of norcorrole **1** resulted in a substantial reduction in its HOMO–LUMO gap.



REFERENCES

1. Kino, S.; Ukai, S.; Fukui, N.; Haruki, R.; Kumai, R.; Wang, Q.; Horike, S.; Phung, Q. M.; Sundholm, D.; Shinokubo, H. *J. Am. Chem. Soc.* **2024**, *146*, 9311.
2. Ishikawa, S.; Yamasumi, K.; Sugiura, S.; Sato, S.; Watanabe, G.; Koo, Y. H.; Seki, S.; Bando, Y.; Haketa, Y.; Shinokubo, H.; Maeda, H. *Chem. Sci.* **2024**, *15*, 7603.

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Photoredox Reactions Mediated by Corrole Derivatives

Ashmita Jain[a], Iti Gupta*[a]

[a] *Department of Chemistry, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar-382355, Gujarat, India. *E-mail: jainashmita@iitgn.ac.in, iti@iitgn.ac.in*

Visible light, an abundant and sustainable energy source, can be used to accelerate organic transformations of molecules *via* a photocatalyst. Typically, Ru(II) and Ir(III) polypyridyl complexes, as well as organic dyes, have been utilised for photocatalyzed organic transformations.[1] Corroles are tetrapyrrolic macrocycle that owes their name to the corrin ring found in Vitamin B12.[2] Compared to porphyrin, it has one less methine bridge and is a tridentate ligand. Corrole exhibits attractive photophysical and electrochemical properties compared to porphyrin and thus should be an excellent photocatalyst. Metallo-corroles have found applications in water splitting, CO_2 reduction, the synthesis of novel solar cells, and various organic transformations, such as epoxidation, cyclopropanation, and sulfoxidation.[3] However, the photocatalytic applications of corrole are still underexplored.

Our group at IIT Gandhinagar is working on the photocatalytic applications of corroles, porphyrins, and metal dipyrrinato complexes [4]. This poster presents the synthesis and characterization of a series of A_2B-type metallo-corroles having heterocyclic moieties at their *meso*-positions. The work describes a non-toxic, efficient method for the synthesis of benzimidazoles via visible-light-induced condensation cyclisation of aromatic aldehydes and *o*-phenylenediamines, using metallo-corrole as a photocatalyst. The desired products were obtained in good yields. The results of TD-DFT calculations will also be discussed to explain the reaction mechanism.

REFERENCES

1. Narayanam, J. and Stephenson, C. Chemical Society Reviews, **2011**, *40*, 102-113 .
2. Iris, A. and Gross, Z Chemistry A European Journal, **2009**, *15*, 8382–8394.
3. Jain, A.; Kumar, S.; Sanyam.; Mondal, A.; and Gupta, I. Journal of Catalysis. **2024**, *438*, 115705
4. Janaagal, A.; Sanyam; Mondal, A.; and Gupta, I. Journal of Organic Chemistry **2023**, *88*, 9424-9431

POSTERS

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Photo-activated Adipose-Derived Stem Cells with Improved Paracrine Immunomodulation for Inflammatory Bowel Disease

Yu Min Jang[a,b] and Kun Na[a,b,*]

[a] *Department of Biomedical-Chemical Engineering, The Catholic University of Korea*
[b] *Department of Biotechnology, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Bucheon-si, Gyeonggi-do 14662, Republic of Korea*

Inflammatory bowel disease (IBD) is a chronic inflammatory disease, and current immunosuppressant and biological drug treatments have limitations such as side effects, incomplete reactions, and resistance.[1] Among them, adipose-derived stem cells (ADSC) exhibit potent immunomodulatory effects, but their therapeutic potential is limited by reduced survival and decreased anti-inflammatory paracrine secretion in inflammatory environments.[2, 3]

To solve the limitations of ADSC, polyethylene glycol-chlorin e6 (PC) was conjugated with cyclic imide-PC (CPC), and an integrin-binding peptide was added to produce integrin-binding peptide (ICPC) to specifically bind to ADSC's integrin receptor. Then, AICPC was developed as ICPC-labeled ADSCs. By manufacturing AICPC compared to the existing ADSC, light-induced reactive oxygen species (ROS) were used as a stimulus to activate intracellular signaling and enhance the survival and anti-inflammatory paracrine secretion of ADSC. It was proven that ICPC was synthesized by confirming its structural properties and molecular weight via spectroscopic and mass spectrometry-based analyses, and flow cytometry was used to demonstrate that it specifically binds to ADSC compared to other cell lines. *In vitro,* cell stimulation was confirmed by ROS generation upon irradiation with a 671 nm laser (0.5 J/cm²). Afterwards, an enzyme-linked immunosorbent assay confirmed that AICPC increased transforming growth factor-beta (TGF-β) and interleukin-10 (IL-10) and reduced pro-inflammatory cytokines in lipopolysaccharide-macrophage co-culture, and photo-activated AICPC induced an anti-inflammatory immune microenvironment by increasing anti-inflammatory and regenerative factors and exosome secretion. In IBD mice induced with dextran sulfate sodium *in vivo*, AICPC improved weight loss and the disease activity index and restored colon length. It also decreased pro-inflammatory cytokines and showed systemic immunomodulatory and intestinal tissue protection effects by increasing IL-10 and TGF-β levels and reducing effector memory $CD8^+$ T cells.

Based on these effects, AICPC, which reprogrammed ADSC paracrine signaling toward anti-inflammatory and regenerative effects via integrin targets and photoinduced ROS, is expected to serve as a stem cell engineering platform for IBD treatment.

REFERENCES

1. Moreno LO, Fernández-Tomé S, Abalo R. Biological Treatments in Inflammatory Bowel Disease: A Complex Mix of Mechanisms and Actions. *Biologics*. 2021; 1(2):189-210.
2. Na Song, Martijn Scholtemeijer, Khalid Shah, Mesenchymal Stem Cell Immunomodulation: Mechanisms and Therapeutic Potential, Trends in Pharmacological Sciences, 41, 9, (2020): 653-664,
3. Dabrowska S, Andrzejewska A, Janowski M and Lukomska B, Immunomodulatory and Regenerative Effects of Mesenchymal Stem Cells and Extracellular Vesicles: Therapeutic Outlook for Inflammatory and Degenerative Diseases. *Front. Immunol.* 11, (2021):591065

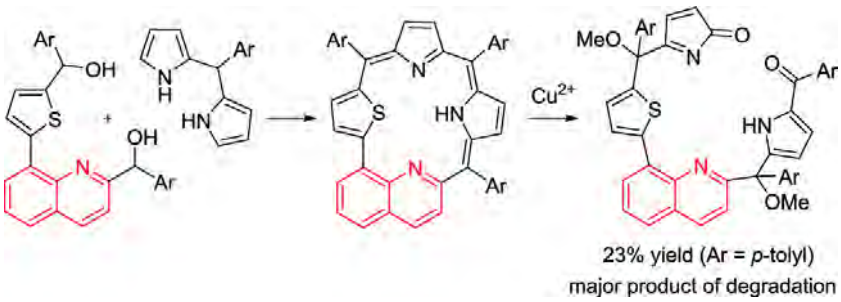
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Quinoliporphyrin as an Aromatic Monoanionic Porphyrinoid and Its Degradation Promoted by Cu^{2+}

Hyeon-Seok Jeong, Yoon-Hee Lee, Sung-Wook Choi, Dong-Gyu Cho*

Department of Chemistry and Chemical Engineering, Inha University



This study presents the first synthesis and characterization of quinoliporphyrin[1], a unique aromatic monoanionic macrocycle featuring a quinoline unit within the porphyrinoid core. Previously, quinoline-containing porphyrins had their quinoline units positioned at peripheral locations[2]. This structural feature exhibits exclusive reactivity with Cu^{2+}, leading to rapid degradation at μM concentrations within 30 min at room temperature and the formation of a fluorogenic product. Such mild and rapid reactivity is attributed to the presence of the quinoline core[3].

REFERENCES

1. Szyszko, B.; Białek, M. J.; Pacholska-Dudziak, E.; Latos-Grażyński, L. Flexible Porphyrinoids. *Chem. Rev.* **2017**, *117*, 2839– 2909
2. Akhigbe, J.; Luciano, M.; Zeller, M.; Brückner, C. Mono- and Bisquinoline-Annulated Porphyrins from Porphyrin β,β′-Dione Oximes. *J. Org. Chem.* **2015**, *80*, 499– 511
3. Furuta, H.; Maeda, H.; Osuka, A. Regioselective Oxidative Liberation of Aryl-Substituted Tripyrrinone Metal Complexes from N-Confused Porphyrin. *Org. Lett.* **2002**, *4*, 181– 184

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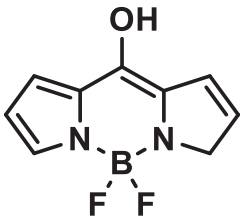


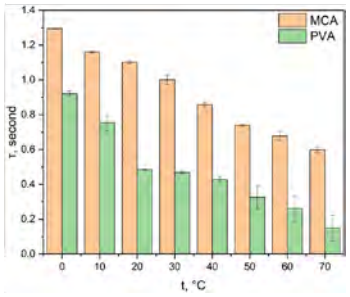
Ultralong Room-Temperature Phosphorescence of BODIPY Dye into Matrix

Alexander A. Kalyagin[a], Alexander A. Goncharenko[a, b], Daniil N. FInogenov[b], Alexander A. Ksenofontov[a], Elena V. Antina[a], Mikhail B. Berezin[a], Pavel A. Stuzhin[b]

[a] *Institute of Solution Chemistry, Russian Academy of Sciences, Academic St. 1, Ivanovo, 153045*
[b] *Research Institute of Macroheterocyclic Compounds, Ivanovo State University of Chemistry and Technology, Sheremet'evskiy av. 7, Ivanovo, 153000*

BODIPY (boron-dipyrromethene) dyes have long been established as highly efficient fluorescent labels, with quantum yields approaching unity [1].
For many years, the direct observation of BODIPY phosphorescence was only possible in rigid glassy matrices at cryogenic temperatures (78 K) and required the incorporation of heavy atoms (e.g., bromine) to enhance spin-orbit coupling [2].
A groundbreaking study by an international team of researchers [3] challenged the established notion regarding the impossibility of triplet state generation in heavy-atom-free BODIPY chromophores. The authors discovered significant delayed emission (on the microsecond timescale) in solutions of commercial BODIPY dyes that lacked heavy metal atoms.





The key achievement of this work was an absolutely unique finding is the observation of ultralong room-temperature phosphorescence (URTP) in simple BODIPY.
This work will demonstrate materials incorporating a peripherally unsubstituted meso-hydroxy BODIPY in matrices of various natures, as well as the influence of the environment (temperature, humidity) on the phosphorescence properties. The incorporation of the dye into matrices has enabled outstanding phosphorescence lifetime results, ranging from 0.5 to 1.5 seconds at room temperature, which represent a record value for this class of compounds.
Thus, this research not only revises the fundamental photophysical understanding of BODIPY dyes but also opens new avenues for creating highly efficient materials with long-lived phosphorescence for applications in bioimaging, organic electronics, and photodynamic therapy.
The report will be of interest to anyone interested in phosphorescent materials and the methodology for studying these properties.

This work was supported by the Russian Science Foundation (grant RSF 24-73-00309).

REFERENCES

[1] N. A. Bumagina, et al., *Coordination Chemistry Reviews*, **2022**, *469*, 214684.
[2] X.F. Zhang, et al., *Journal of Photochemistry and Photobiology A: Chemistry*, **2014**, *285*, 16–20.
[3] E. Rebollar, et al., *Molecules*, **2022**, *27 (15)*, 4683.

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Helical and Nanoparticle Structures in Self-Assembled Porphyrin Dyads by Linker Modification

Dae Eun Kang[a], Woo-Dong Jang[a]

[a]*Department of Chemistry, Yonsei University, Seoul, Republic of Korea*

Porphyrin dyads are versatile building blocks for supramolecular polymers because their planar π-surfaces promote directional intermolecular interactions while allowing structural variation. Nevertheless, controlling the morphology of Zn-centered porphyrin dyads has often remained difficult. In our previous studies, Zn dyads tended to assemble in a largely uncontrolled manner and frequently formed particle-like aggregates, suggesting that strong metal–metal (Zn–Zn) association can dominate the packing landscape and obscure rational morphology selection. [1-2]

In this work, we designed and synthesized a series of compounds in which the inter-porphyrin connector was varied from phenylene (Ph) to biphenylene (BP) and triphenylene (TP), denoted as Linker–DPDZn and Linker–TPDZn (e.g., Ph–DPDZn, TP–TPDZn). Self-assembly was investigated in methylcyclohexane under thermodynamically stable cooling conditions (1 K/min) using temperature-dependent UV–Vis spectroscopy and morphology characterization.

Across the series, the aggregation morphology was found to change with linker length. The results indicate that linker-dependent changes in the distance and relative orientation of the two porphyrin units modulate the balance between competing packing modes, leading to the selective formation of fibrous or particle-like aggregates. Overall, these findings demonstrate that varying aromatic linker length provides a straightforward basis for achieving morphology control in Zn porphyrin dyads.

REFERENCES

1. Lee, H.; Lee, M.; Hwang, J. H.; Kim, I.; Lee, E.; Jang, W.-D. Recognition of Atomic-Level Difference in Porphyrin Dyads for Self-Sorted Supramolecular Polymer Growth. Nanoscale 2023, 15 (45), 18224–18232. https://doi.org/10.1039/d3nr04851a.
2. Lee, H.; Lee, Y.; Lee, M.; Kang, D. E.; Kim, J.; Kim, D. H.; Jang, W. Pathway Complexity in Supramolecular Polymerization of Porphyrin Dyads for Kinetic Control of Helicity. Aggregate 2025, 6 (8). https://doi.org/10.1002/agt2.70090.

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It can be whatever you want: The reactivity of tellurophene embedded in the porphyrinoid skeleton toward osmium carbonyl

Dominika Kasperek[a], Ewa Pacholska-Dudziak[a]

[a] *University of Wrocław, Faculty of Chemistry, F. Joliot-Curie 14, 50-383 Wrocław, e-mail: dominika.kasperek@uwr.edu.pl*

Telluraporphyrinoids are heteroporphyrins in which at least one pyrrole ring has been replaced with a tellurophene ring. Due to the presence of a relatively weak C–Te bond, these macrocycles exhibit unusual and interesting reactivity. When telluraporphyrinoids react with metal ions, in addition to classic metal complexes, *metallaporphyrins* are formed [1-4]. In *metallaporphyrins*, a metal atom replaces the tellurium atom. The chlorination of telluraporphyrinoids results in the oxidation of the tellurium atom and the attachment of two chloride ligands [5,6]. Under acidic conditions at high temperatures, the tellurium atom is removed from the macrocyclic skeleton, and the tellurophene unit is transformed into the butadiene unit [7,8].

Here we present the results of our research on the reactivity of various telluraporphyrinoids toward triosmium dodecacarbonyl [$Os_3(CO)_{12}$]. In addition to the expected replacement of tellurium atom(s) with osmium atom(s), the following occurred: osmium atom(s) were incorporated into the C-Te bond to form a six-membered ring; tellurium atom(s) were eliminated from the macrocyclic skeleton to form annulene fragment(s); and most remarkably, an oxo-cyclopentadiene ring formed in place of tellurophene.

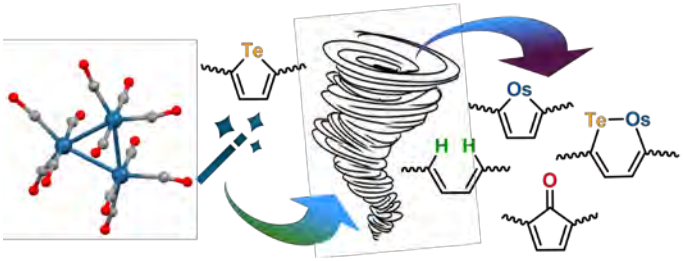


Figure 1. Schematic reactivity of tellurophene incorporated into porphyrins toward osmium carbonyl.

REFERENCES

[1] E. Pacholska-Dudziak, M. Szczepaniak, A. Książek, L. Latos-Grażyński, *Angew. Chem. Int. Ed.* **2013**, 52, 8901-8902.
[2] E. Pacholska-Dudziak, G. Vetter, A. Góratowska, A. Białońska, L. Latos-Grażyński, *Chem. Eur. J.* **2020**, 26, 16013-16015.
[3] G. Vetter, A. Białońska, P. Krzyszowska, S. Koniarz, E. Pacholska-Dudziak, *Chem. Eur. J.* **2022**, 28, e202202167.
[4] G. Vetter, A. Białońska, A. Jezierska, J. J. Panek, E. Pacholska-Dudziak, *Chem. Commun.* **2023**, 59, 6841-6844.
[5] M. Abe, M. R. Detty, O. O. Gerlits, D. K. Sukumaran, *Organometallics* **2004**, 23, 4513–4518.
[6] P. Krzyszowska, E. Ganczar, P. J. Chmielewski, E. Pacholska-Dudziak, *Inorg. Chem.* **2024**, 63, 21788-21800.
[7] E. Pacholska, L. Latos-Grażyński, Z. Ciunik, *Chem. Eur. J.* **2002**, 8, 5403-5406.
[8] E. Pacholska-Dudziak, L. Latos-Grażyński, A. Białońska, *Chem. Eur. J.* **2019**, 25, 10088-10097.

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Heteroleptic Iridium Complexes show unmatched potency as antimicrobial photosensitizers for hard-to-treat bacterial and fungal infections

Giulia Kassab[a], Caitlyn Lee[a,b], Juan Chen[a], Wenfang Sun[c], Gang Zheng[a,d]

[a]*Princess Margaret Cancer Center, University Health Network, Toronto, ON, Canada;*
[b]*Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON, Canada;*
[c]*Department of Chemistry and Biochemistry, University of Alabama, Tuscaloosa, AL, USA;*
[d]*Department of Medical Biophysics, University of Toronto, Toronto, ON, Canada*

Antimicrobial resistance is estimated to surpass cancer as a cause of mortality and be responsible for over 10 million deaths worldwide by 2050 [1-2]. Antimicrobial photodynamic therapy (aPDT) evades the development of resistance and has the potential to convert resistant strains into susceptible ones. However, aPDT has found limited translation into clinical settings. Here, we present metal-complex-based photosensitizers that show unmatched potency against hard-to-treat pathogens. The gram-negative *Pseudomonas aeruginosa* is classified as a high-priority bacterial pathogen and is often associated with antibiotic resistance [3-4]. The heteroleptic Iridium complex 3T-Ir inactivates about 7 log of *P. aeruginosa* at as little as 1 μM and 10 J/cm², being 100 times more potent than Rose Bengal (RB) in a direct comparison and more potent than any other photosensitizer reported in the literature. In biofilm conditions, as little as 10 μM and 10 J/cm² are sufficient to decrease viability by over 90%. And in a mouse model of skin wound infection, 3T-Ir not only outperforms RB, but also the gold-standard antibiotic levofloxacin, in reducing infection burden. *Candidozyma auris* is an emerging multi-drug-resistant fungal pathogen [5], for which a similar 100-fold difference in potency to RB, and no match in the literature has been found for the complex 4T-Ir when *in vitro*. In such a case, only 100 nM and 10 J/cm² are necessary, and these same conditions are sufficient to reduce viability by 80% in a *C. auris* biofilm. Overall, 3T-Ir and 4T-Ir show tremendous potential as aPDT agents and could help address the urgent need to overcome antimicrobial resistance.

REFERENCES

1. C. J. Murray *et al.*, "Global burden of bacterial antimicrobial resistance in 2019: a systematic analysis," *Lancet*, vol. 399, no. 10325, pp. 629–655, 2022, doi: 10.1016/S0140-6736(21)02724-0.
2. J. O'Neill, "Tackling Drug-Resistance Infections Globally: Final Report and Recommendations. The review on Antimicrobial Resistance," 2016. [Online]. Available: https://amr-review.org/sites/default/files/160518_Final paper_with cover.pdf
3. World Health Organization, *WHO Bacterial Priority Pathogens List, 2024: bacterial pathogens of public health importance to guide research, development and strategies to prevent and control antimicrobial resistance*. Geneva, 2024.
4. S. Bertagnolio *et al.*, "WHO global research priorities for antimicrobial resistance in human health," *The Lancet Microbe*, vol. 5, no. 11, pp. 1–14, 2024, doi: 10.1016/S2666-5247(24)00134-4.
5. World Health Organization, *WHO fungal priority pathogens list to guide research, development and public health action.*, vol. 1. 2022.

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Symmetry Breaking Charge Separation in Zinc Phthalocyanine Dimers Self-Assembled via Hydrogen Bonding

Ram R. Kaswan[a], Lydia Ferrer-López[b], Desire Molina Alcaide[b], Ángela Sastre-Santos*[b], Francis D'Souza*[a]

[a]*Department of Chemistry, University of North Texas at Denton, 1155 Union Circle, #305070, Denton, TX 76203-5017 (USA)*
[b]*Área de Química Orgánica, Instituto de Bioingeniería, Universidad Miguel Hernández, Avda. de la Universidad s/n 03203 Elche (Spain)*

Photoinduced symmetry-breaking charge separation (SB-CS) in a symmetrical pair of dimers is known to maximize energy conversion during the light-to-chemical energy conversion process [1]. Although this has been shown in a few covalently linked dimers [2], the demonstration of such an event in self-assembled chromophore dimers has been very rare [3], especially in dimers formed by hydrogen bonding interactions. Here, we present a classic example of hydrogen bonding paired self-assembled zinc phthalocyanine dimers ((ZnPc-COOH)$_2$ and (ZnPc-Ph-COOH)$_2$) of different chromophore distances and demonstrate SB-CS resulting in ZnPc$^{\bullet+}$-ZnPc$^{\bullet-}$ electron transfer products upon far-red light illumination. The occurrence of SB-CS in the ZnPc-dimers was confirmed by multiple studies, including fluorescence emission, which showed significant quenching in the dimer compared to analogous monomers. Estimation of energy stored in the charge-separated states from electrochemical studies (redox gap of ~1.55 eV) revealed the energy to be close to the pumping energy ($E_{0,0}$ ~ 1.80 eV), thus minimizing the energy loss during light-to-energy conversion. While DFT studies assessed the geometry and carboxylic acid pairing strength, TD-DFT studies identified the excited states responsible for promoting excited-state electron transfer within the ZnPc dimers. Finally, femtosecond pump–probe studies provided definitive evidence of SB-CS, with electron transfer rate constants of 5×10^{11} and 0.7×10^{11} s^{-1}, respectively, for (ZnPc-COOH)$_2$ and (ZnPc-Ph-COOH)$_2$, revealing the significance of H-bond-pairing in promoting efficient charge separation in the far-red capturing ZnPc dimers.

REFERENCES

1. R. R. Kaswan, A. Yahagh, F. D'Souza, *Chem. Sci.* **2026**, Accepted Manuscript.
2. R. R. Kaswan, D. Molina, L. Ferrer-López, J. Ortiz, P. A. Karr, Á. Sastre-Santos, F. D'Souza, *Angew. Chem. Int. Ed.* **2025**, *64*, e202502516
3. R. R. Kaswan, L. Ferrer-López, D. M. Alcaide, Á. Sastre-Santos, F. D'Souza, *J. Am. Chem. Soc*. **2025**, *147*, 46766–46772.

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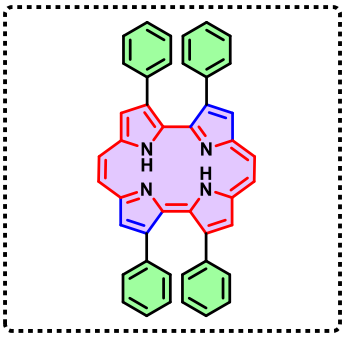


3,6,13,16-Tetraarylporphycene: A New Class of Porphycene Derivative Exhibiting Atropisomerism

Katari Narmada[a], Pradeepta K. Panda*

[a]*School of Chemistry, University of Hyderabad, Hyderabad – 500 046, India. E-mail: narmada054@gmail.com*

Porphycene, the first abiotic constitutional isomer of porphyrin, was reported in 1986 by Vogel and coworkers and features a rectangular macrocyclic core stabilized by strong intramolecular NH···N hydrogen bonding[1]. Synthesis of 3,6,13,16-tetrasubstituted porphycenes eluded chemists for more than three decades, until our group's recent reports of 3,6,13,16-tetramethoxyporphycene and 3,6,13,16-tetraalkylporphycene revealed a square-type core and fluorescence [2]. These macrocycles formed complexes with various metal ions and undergo facile tetra-halogenation at the outer β-positions, e.g., bromination. Herein, we report the **first synthesis and structural investigation of 3,6,13,16-tetraphenylporphycene**. This novel derivative was designed to probe the stereoelectronic influence of aryl groups and to evaluate the possibility of atropisomerism arising from restricted rotation about the macrocycle–aryl σ-bonds. Single-crystal X-ray diffraction analysis of an isolated fraction reveals distinct phenyl orientations, allowing unambiguous correlation with a specific atropisomeric conformer **(ααββ)**. This modulates the porphycene core to enable efficient metal coordination, as evidenced by smooth palladium metalation. Unlike meso-substituted porphyrins[3], porphycenes had not exhibited atropisomerism. This study provides the **first structural evidence of atropisomerism in aryl-substituted porphycenes**, expanding their conformational and functional scope.



REFERENCES

1. Vogel, E.; Kocher, M.; Schmickler, H.; Lex, J. Porphycene-a novel porphin isomer. *Angew. Chem., Int. Ed. Engl*. **1986**, *25*, 257−259.
2. (a) Rana, A.; Kumar, B. S.; Panda, P. K. 3,6,13,16-Tetrasubstituted Porphycene. *Org. Lett*. **2020**, *22*, 7175−7180. (b) Nagamaiah, J.; Dutta, A.; Pati, N. N.; Sahoo, S., Soman, R.; Panda, P. K. 3,6,13,16-Tetrapropylporphycene: Rational synthesis, Complexation and Halogenation. *J. Org. Chem.* **2022**, *87*, 2721-2729. 3. Gottwald, E.; Ullmann, F. Atropisomerism in Mesosubstituted Porphyrins. *Chem. Ber.* **1969**, *102*, 1533–1542.

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Peroxygenase engineering of bacterial cytochrome P450 CYP107J1 for use as a biocatalyst

Hideki Kato[a], Takafumi Hashimoto[a], Tuhin Das[b], Daniel Z Doherty[b], Stephen G. Bell[b], Toshiki Furuya[a]

[a]*Department of Applied Biological Science, Faculty of Science and Technology, Tokyo University of Science, Japan*
[b]*Discipline of Chemistry, School of Physics, Chemistry and Earth Sciences, Adelaide University, Australia*

Cytochrome P450 monooxygenases (P450s) are a superfamily of heme-containing enzymes that introduce a single oxygen atom from molecular oxygen into organic compounds. *Bacillus subtilis* strain 168, a model bacterium, possesses eight P450 genes, but the catalytic function of CYP107J1 remains to be fully elucidated [1]. Previous studies failed to identify the genes encoding the reductase component required for CYP107J1 activity from the genome sequence. Therefore, we reconstituted the enzyme activity of CYP107J1 using putidaredoxin (Pdx) and its reductase (PdR) from *Pseudomonas putida*, a well-studied reductase component. The enzyme exhibited oxidation activity toward 4-alkylbenzoic acids with carbon chain lengths of 3 to 8, although the activity was low [2]. This is possibly caused by the use of heterologous redox partners. Recently, Bell and coworkers modified the bacterial P450 CYP199A4 to a hydrogen peroxide (H_2O_2)-driven form (i.e., a peroxygenase) that does not require redox partners by replacing the T252 residue with Glu. The introduced Glu residue at position 252 binds a water molecule near the heme, acting as an acid-base catalyst and enabling the generation of Compound I from H_2O_2. The peroxygenase activity of the resulting T252E mutant was dramatically increased by the further introduction of a D251Q mutation [3]. In this study, we engineered CYP107J1 to function as a peroxygenase to enhance its low activity.

CYP199A4 residues D251 and T252 correspond to E251 and T252 of CYP107J1. Structural analysis of CYP107J1 using AlphaFold 3 revealed that E251 and T252 are located near the heme moiety. We therefore constructed a E251Q/T252E double mutant (CYP107J1-QE). The QE mutant exhibits peroxygenase activity toward 4-alkylbenzoic acids with a carbon chain length of 3 to 7, similar to the monooxygenase activity of the wild-type enzyme. The QE mutant exhibited the highest peroxygenase activity toward 4-hexylbenzoic acid (50.7 mol-P450^{-1} min^{-1}), which was 28 times higher than the monooxygenase activity of the wild-type enzyme supported by Pdx and PdR (1.8 mol mol-P450^{-1} min^{-1}). Interestingly, the engineered enzyme not only oxidized 4-alkylbenzoic acids, it also efficiently produced the valuable dye indigo by simply mixing the enzyme with indole and H_2O_2. The QE mutant produced indigo at 30 mol mol-P450^{-1} min^{-1} in the presence of 20 mM H_2O_2, with an indigo yield of 0.15 mM (39 mg L^{-1}) in 10 min. These results indicate that CYP107J1-QE is a superior biocatalyst for indigo synthesis using H_2O_2 as the oxidant.

REFERENCES

1. Furuya T, Nishi T, Shibata D, Suzuki H, Ohta D, Kino K, *Chem Biol*, 15:563-572 (2008).
2. Furuya T, Kato H, Bell SG, 20th International Conference on Biological Inorganic Chemistry (ICBIC20) (abstract p.370), Adelaide, Australia, 16-21 July 2023.
3. Podgorski MN, Akter J, Churchman LR, Bruning JB, De Voss JJ, Bell SG, *ACS Catal,* 14:7426-7443 (2024).

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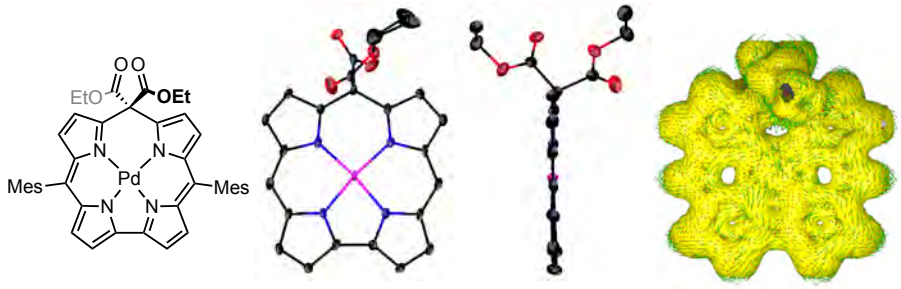


Synthesis and Properties of 10-Isocorrole Metal Complexes

Satoshi Kato[a], **Hideaki Takano**[a,b], **Hiroshi Shinokubo**[a]

[a]*Department of Molecular and Macromolecular Chemistry, Graduate School of Engineering, Nagoya University, Chikusa-ku, Nagoya464-8603, Japan*
[b]*Institute for Advanced Research, Nagoya University, Chikusa-ku, Nagoya 464-8601, Japan*

Isocorroles exhibit characteristic near-infrared absorption properties, high singlet oxygen sensitization ability,[1] and high photothermal conversion efficiency.[2] In addition, theoretical calculations suggest that isocorroles display either homoaromatic or homoantiaromatic character depending on the substituents at the saturated *meso* position.[3] To date, isocorroles have been synthesized as mixtures of isomers via nucleophilic addition to triarylcorroles.[4] Herein, we synthesized 10-isocorrole metal complexes selectively via S_NAr reaction of carbon nucleophiles to tetraphyrin derivatives. The structures of the obtained 10-isocorroles were determined by the X-ray diffraction analysis. They have high planar frameworks, including a saturated carbon center at the *meso* position. Electrochemical measurements and absorption spectroscopy revealed their narrow HOMO–LUMO gaps. In addition, ^{1}H NMR spectroscopy and theoretical calculations suggested their weak homoaromatic character.



REFERENCES

1. Larsen, S.; Adewuyi, J. A.; Ung, G.; Ghosh, A. *Inorg. Chem.* **2023**, *62*, 7483–7490.
2. Caine, J. R.; Larsen, S.; Ghosh, A.; Hudson, Z. M. *Inorg. Chem.* **2025**, *64*, 1246–1251.
3. Foroutan-Nejad, C.; Larsen, S.; Conradie, J.; Ghosh, A. *Sci Rep*. **2018**, *8*, 11952.
4. Nardis, S.; Pomarico, G.; Mandoj, F.; Fronczek, F. R.; Smith, K. M.; Paolesse, R. *J. Porphyr. Phthalocyanines* **2010**, *14*, 752–757.

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Curvature-Driven Supramolecular Polymerization of a Porphyrin Dyad with a Scissor-Shaped Motif

Ryuichi Kawai[a], Soichiro Ogi[b], Hiroki Hanayama[c] and Shiki Yagai[c, d]

[a] *Division of Advanced Science and Engineering, Graduate School of Engineering, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan.*
[b] *Integrated Research Consortium on Chemical Science (IRCCS), Nagoya University, Furo, Chikusa, Nagoya 464-8682, Japan.*
[c] *Department of Applied Chemistry and Biotechnology, Graduate School of Engineering, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan.*
[d] *Institute for Advanced Academic Research (IAAR), Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan.*

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Curvature has recently been recognized as a key structural parameter that defines the pathway and topology of supramolecular polymerization. However, this perspective has remained relatively unexplored because only a limited number of molecular systems can precisely induce the diverse curved structures such as rings, helicoids, and tubes.[1] We previously reported that scissor-shaped azobenzene dyads, linked as dimers through a xylylene spacer bearing long alkyl chains, undergo folding-driven self-assembly to form curvature-derived architectures such as nanorings and nanotubes.[2] Herein, we extend this scaffold to a bulkier chromophore and demonstrate that the curvature-directed pathway remained intact. To this end, we synthesized the scissor-shaped tetraphenylporphyrin dyad **1** (Figure 1a) and investigated its self-assembly.

Upon cooling a hot monomeric solution of **1** in nonpolar solvent, AFM observation revealed that **1** formed ill-defined structures (Figure 1b). After aging this solution for 1 day, AFM imaging showed that **1** self-assembled into helicoidal supramolecular polymers (Figure 1c). Further aging of this solution resulted in the transition into nanotubes over 140 h. On the other hand, applying sonication beforehand induces fragmentation that closes the curved segments into discrete rings (Figure 1e). Therefore, we demonstrated that the scissor-shaped molecular design is a promising strategy to self-assemble bulkier chromophores into well-defined curved nanostructures.[3]

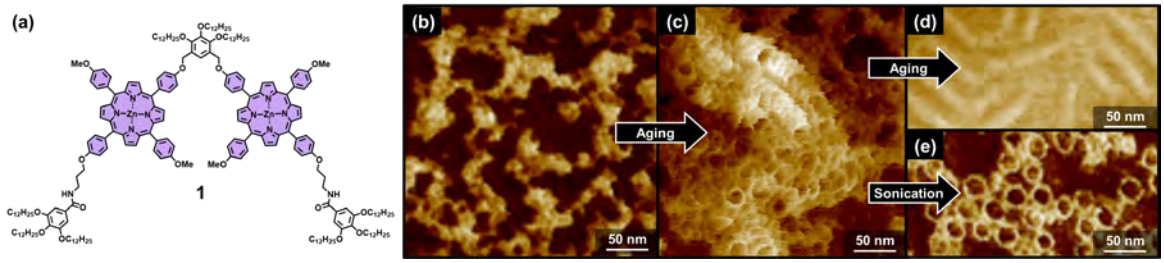


Fig. 1 (a) Molecular structure of **1**. (b–e) AFM images of (b) ill-defined structures, (c) helicoids, (d) tubes and (e) rings of **1**.

REFERENCES

1. H.-X. Wang, X. Zhu and M. Liu, *Chem. Soc. Rev.*, **2025**, 54, 5516–5550.
2. T. Saito, T. Kajitani and S. Yagai, *J. Am. Chem. Soc.*, **2023**, 145, 443–454.
3. R. Kawai, S. Ogi., H. Hanayama, R. Kudo and S. Yagai, *Chem. Sci.*, **2026**, 17, 2559–2565.

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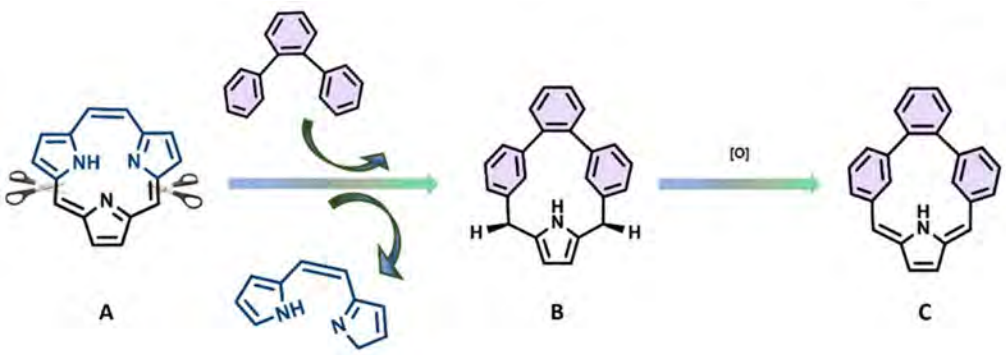


Dicarbatriphyrin(2.1.1) and Carbacalix[1]phyrin(2.*1.1*) analogue: Structure-property relationship and application as a Fe(III) chemosensor

Adrija Kayal[a], **Mainak Das**[b], **A. Srinivasan**[a]

[a]*School of Chemical Sciences, National Institute of Science Education and Research (NISER), An OCC of Homi Bhabha National Institute, Bhubaneswar 752050, Odisha (India).*
[b]*Sorbonne Université, CNRS, Institut Parisien de Chimie Moléculaire, IPCM, Paris 75005, France.*

Porphyrinoid macrocycles possess versatile frameworks that enable systematic exploration of π-electron delocalization via topological modifications. This strategic design can induce several properties, such as i) tunable optoelectronic behaviour[1a], ii) aromaticity switching[1b], and iii) small molecule sensing ability[1c]. The core size of such porphyrinoids has been reported to play a crucial role in determining their structural and functional properties. For example, the introduction of a carbocyclic moiety in the triphyrin core, a contracted porphyrinoid with three pyrrole units in the core[2] (**A**), alters the macrocyclic topology and influences the stability of the core as well. Such carbatriphyrins reported to date have either been isolated as their protonated form[3] or obtained as organophosphorous, i.e., P(V) complex[4]. In this poster, we present the synthesis and characterization of two such π-extended macrocycles, carbacalix[1]phyrin(2.*1.1*) (**B**) and its oxidised analogue, dicarbatriphyrin (2.1.1) (**C**). The arrangement of the phenyl rings within the macrocyclic scaffolds was found to dictate the chair conformation in **B**. Whereas, **C** adapted a saddle shape with a negative Gaussian curvature arising from its unique topology. Notably, **C** displayed intense fluorescence in the solution state, which was selectively quenched in the presence of Fe (III) ions. This curvature-controlled molecular sensing behaviour highlights **C** as a potential chemo-sensor for ferric ions.[5]



REFERENCES

1. a) C. Qu, X. Gong, Y. Sun, H. Gao, F. Cai, Y. Zhao, F. Wu, Z. Shen, *Chem. Sci*., **2024**, *15*, 10491-10498; b) M. C. Yoon, P. Kim, H. Yoo, S. Shimizu, T. Koide, S. Tokuji, S. Saito, A. Osuka, D. Kim, *J. Phys. Chem*., **2011**, *115*, 14928-14937; c) P. S. Salini, M. G. D. Holaday, M. L. P. Reddy, C. H. Suresh, A. Srinivasan, *Chem. Commun.*, **2013**, *49*, 2213-2215.
2. K. S. Anju, S. Ramakrishnan, A. Srinivasan, *Org. Lett*., **2011**, *13*, 2498-2501.
3. M. Pawlicki, M. Garbicz, L. Szterenberg, L. Latos-Grażyński, *Angew. Chem. Int. Ed*., 2015, **54**, 1906–1909.
4. A. Kumar, K. G. Thorat, A. Sinha, R. J. Butcher, M. Ravikanth, *J. Org. Chem*., 2019, **84**, 9067–9074.
5. A. Kayal, S. R. Pradhan, C. K. Prasad, M. Das, A.Srinivasan, *Chem. Asian J*., **2024**, e202401089.

POSTERS

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Overcoming Delivery Barriers Using a Customized Photo-Activated Polyplex for Intranasal mRNA Delivery

Yeong A Kim [a, b], **Kun Na** [a, b *]

[a] *Department of Biomedical-Chemical Engineering, The Catholic University of Korea*

[b] *Department of Biotechnology, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Bucheon-si, Gyeonggi-do 14662, Republic of Korea, E-mail: kna6997@catholic.ac.kr*

The nasal mucosa serves as the first line of defense against external pathogens. It has gained attention as a vaccine delivery route due to its ability to effectively induce both mucosal and systemic immune reponses through the lymphocyte-rich nasal associated lymphoid tissue (NALT) [1]. However, intranasal (IN) mRNA delivery is limited by several structural and biological barriers. These include mucociliary clearance, low absorption efficiency, and endosomal sequestration. These barriers collectively reduce mRNA bioavailability, thereby impairing immune induction efficacy [2].

To overcome these challenges, we designed a customized cationic polyplex(CC_polyplex) incorporating photo-responsive functionality. This system was developed to enhance intranasal mRNA delivery efficiency and immune activation. The CC_polyplex was formulated using a cationic polymer(CC_polymer) with an optimized degree of amine substitution. A photoresponsive moiety was conjugated to enable photo-triggered activation. Upon light irradiation, the system generates reactive oxygen species (ROS). These ROS facilitate endosomal escape and promote cytosolic mRNA release. CC_polyplex significantly increased *in vitro* mRNA delivery efficiency under laser irradiation. After intranasal administration, laser-dependent increases in mRNA expression were observed in both nasal and lung tisseus. The improved delivery efficiency led to enhanced T cell responses and antigen-specific immune response. In particular, antigen-specific IFN-γ secretion from splenocytes was significantly increased. Collectively, these findings demonstrate that a light-controlled precision delivery strategy can overcome barriers in IN mRNA delivery. The CC_polyplex platform may be applicable to both prophylactic viral vaccines and therapeutic cancer vaccines.

REFERENCES

1. CAHN, Devorah, et al. Biomaterials for intranasal and inhaled vaccine delivery. *Nature reviews bioengineering*, 2023, 1.2: 83-84.
2. ZHOU, Hui, et al. ROS-responsive nanoparticle delivery of mRNA and photosensitizer for combinatorial cancer therapy. *Nano Letters*, 2023, 23.9: 3661-3668.

POSTERS

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Interfacial Synthesis of Naphthorosarin-based 2D MOF

Yewon Kim, Woo-Dong Jang*

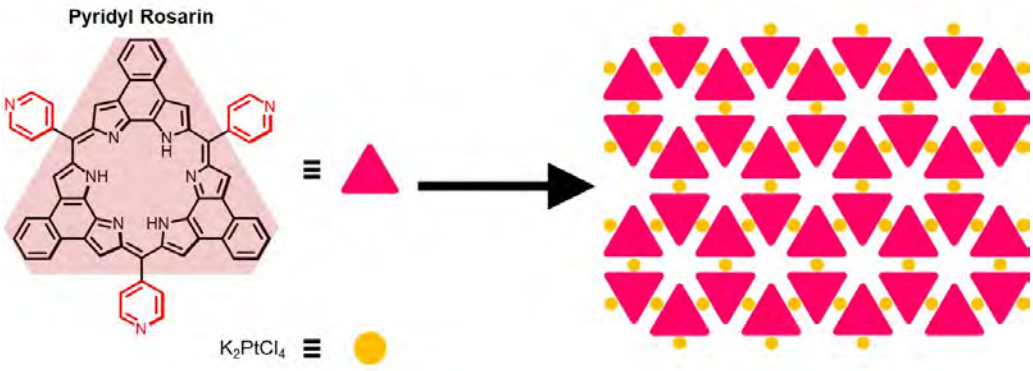
Department of Chemistry, Yonsei University

Metal–organic framework (MOF) thin films have attracted considerable interest due to their structural tunability and versatility in surface-based applications, including sensing, catalysis, and optoelectronics.

In this study, we report the synthesis of a 2D MOF thin film (RoPt MOF) formed through coordination between platinum(II) ions and pyridine-substituted naphthorosarin. Naphthorosarin is a rigid, planar macrocycle featuring a 24 π-electron antiaromatic framework, whose electronic structure can be reversibly modulated via proton-coupled electron transfer (PCET) and redox processes.[1] Although aromatic macrocycles are widely used in framework chemistry, stable antiaromatic systems remain largely unexplored in extended 2D MOF structures.

The RoPt MOF thin film was synthesized via liquid–liquid interfacial approach, enabling directional coordination-driven assembly at the organic–aqueous interface.[2] The square-planar geometry of Pt(II) facilitates predictable coordination with pyridyl ligands, yielding a well-defined layered structure. The resulting film exhibits uniform morphology, as confirmed by AFM and SEM, while XPS verifies the presence of coordination interactions within the MOF structure.

This work demonstrates the successful integration of a planar antiaromatic macrocycle into a 2D MOF thin film and provides a foundation for developing electronically responsive framework materials based on antiaromatic π-systems.



REFERENCES

1. Ishida, M.; Kim, S.-J.; Preihs, C.; Kei Ohkubo; Jong Min Lim; Byung Sun Lee; Jung Su Park; Lynch, V. M.; Roznyatovskiy, V. V.; Sarma, T.; Panda, P. K.; Lee, C.-H.; Shunichi Fukuzumi; Kim, D.; Sessler, J. L. Protonation-Coupled Redox Reactions in Planar Antiaromatic Meso-Pentafluorophenyl-Substituted O-Phenylene-Bridged Annulated Rosarins. *Nature Chemistry* **2012**, 5 (1), 15–20. https://doi.org/10.1038/nchem.1501.

2. Yang, J.; Kong, L.; Huang, C.; Wang, C.; Wei, S.; Zhou, L. Liquid-Liquid Interfacial Approach for Rapid Synthesis of Well-Crystalline Two-Dimensional Metal-Organic Frameworks for Nitro Reduction. *Chemical Engineering Journal* **2024**, 485, 149969. https://doi.org/10.1016/j.cej.2024.149969.

POSTERS

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Boron-Doped Porphyrinoids with Concealed Antiaromaticity

Jonas Klopf, Lukas Swoboda, Manuel Buckel, Holger Helten*

*Julius-Maximilians-Universität Würzburg, Institute of Inorganic Chemistry and Institute for Sustainable Chemistry & Catalysis with Boron (ICB), Am Hubland, 97074 Würzburg, Germany, *holger.helten@uni-wuerzburg.de*

Tuning of the electronic structure of π-conjugated organic materials such as polymers and macrocycles with heteroatoms has become of increasing interest as an efficient means for tailoring their optoelectronic properties for specific applications. Particularly, the incorporation of tricoordinate boron with its vacant p_π orbital opens up new possibilities [1]. We recently presented a series of novel *meso*-boron-doped porphyrinioids (Figure 1) [2-4], including the first globally aromatic boradioxaporphyrin **B₁-C₃-O₂-N₂** (R = Mes*, R' = *p*Tol) [2]. Furthermore, we reported on tetraboratetrathiaporphyrinoid **B₄-S₄** (R = Tip), which shows locally confined aromaticity within its constituent thiophene rings but shows globally concealed antiaromaticity [3]. The equally unprecedented expanded diboratetrathiaporphyrinoid **B₂-C₄-S₄** (R = Mes*), on the other hand, is globally antiaromatic in its neutral form, while after twofold reduction, it switches to the global aromatic dianionic macrocycle **B₂-C₄-S₄²⁻** [4]. This computational work focuses on the predicted photophysical properties and aromaticity of these and further novel porphyrinoid macrocycles.

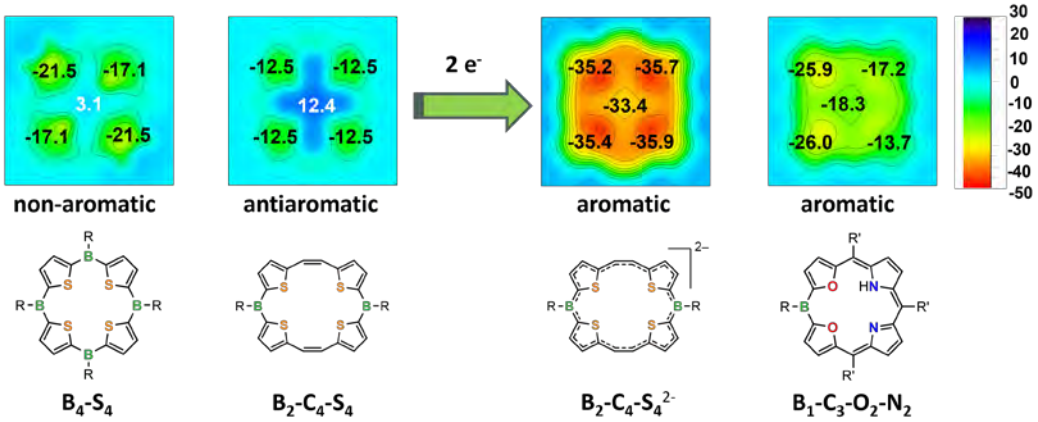


Figure 1: 2D-NICSzz plots of **B₄-S₄**, **B₂-C₄-S₄**, its reduced form **B₂-C₄-S₄²⁻** and **B₁-C₃-O₂-N₂** with R = R' = H.

REFERENCES

1. (a) Yin, X.; Liu, J.; Jäkle, F. *Chem. Eur. J.* **2021**, *27*, 2973−2986. (b) Helten, H. "Organoboron and Related Group 13 Polymers", in *Comprehensive Organometallic Chemistry IV* (Eds.: O'Hare, D.; Meyer, K.; Parkin, G.), Elsevier, New York, 2022, pp. 71–134.
2. Swoboda, L.; Klopf, J.; Fest, M.; Friedrich, A.; Buckel, M.; Krummenacher, I.; Braunschweig, H.; Engels, B.; Helten, H. *J. Am. Chem. Soc.* **2025**, *147*, 10629−10639.
3. Buckel, M.; Klopf, J.; Schneider, J. S.; Lik, A.; Riensch, N. A.; Krummenacher, I.; Braunschweig, H.; Engels, B.; Helten, H. *Nat. Commun.* **2025**, *16*, 1775.
4. Swoboda, L.; Klopf, J.; Buckel, M.; Engels, B.; Helten, H. *J. Am. Chem. Soc.* **2026**, *148*, 2639−2651.

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POSTERS



Photodynamic Inactivation of ESKAPE Pathogens with Novel (Aza)phthalocyanines – Study of Their Activity and Safety

Magdalena Kozlikova[a], Ingrid Hlbocanova[a], Pavlina Vavrova[b], Klara Konecna[b], Miloslav Machacek[a]

[a]*University Affiliation a Faculty of Pharmacy in Hradec Kralove, Department of Biochemical Sciences, Charles University, Czech Republic*
b Faculty of Pharmacy in Hradec Kralove, Department of Biological and Medicinal Sciences, Charles University, Czech Republic

Photodynamic inactivation (PDI) of microorganisms is promising strategy to combat multidrug resistant bacteria. Especially members of the ESKAPE group that pose a major clinical challenge due to their ability to evade conventional antibiotics and frequently cause skin and soft tissue infections. (Aza)phthalocyanines (AzaPcs) offer advantageous photophysical properties and tunable amphiphilicity, making them strong candidates for targeted microbial inactivation in infected wounds [1]. PDI offers a broad spectrum mechanism of action that does not depend on specific molecular targets, which substantially reduces the likelihood of resistance development compared with conventional antibiotics. In addition, PDI is highly effective against microbial biofilms making it a valuable approach for managing chronic, recurrent, and otherwise difficult-to-treat infections [2].
We chose representative charged derivatives that proved to be potential photosensitizers even compared to wide range of different (Aza)Pcs [3]. To evaluate their therapeutic potential and safety, the compounds were tested not only against ESKAPE pathogens but also on normal human fibroblasts, endothelial cells and keratinocytes to assess the risk of local phototoxicity. Because fibroblasts in vivo reside within a complex extracellular matrix rather than a two dimensional monolayer, a 3D model of dermal equivalent composed of fibroblasts embedded in a simulated extracellular matrix was employed to better mimic physiological conditions and to assess the biocompatibility of the treatment in a tissue relevant environment. Antimicrobial activity was evaluated using a recovery based assay (Bioscreen C). The amphiphilic derivative bearing quaternized imidazole-containing moieties was the most potent, achieving complete eradication (MBC) of MRSA at concentrations as low as 100 nM and showing activity (MBC or 3-log reduction) against other ESKAPE strains at higher doses as well. The MBC (minimum bactericidal concentration) of abovementioned derivative did not affect cellular viability in either the 2D or 3D the models. Moreover, all derivatives were unable to penetrate through human skin.

Acknowledgments: Supported by the Ministry of Health of the Czech Republic in cooperation with the Czech Health Research Council under project No.. NW24J-05-00016 and Charles University Grant Agency grant no. 157524.

REFERENCES

1. Yan, E., et al., 2023, *ChemPlusChem.* DOI: 10.1002/cplu.202300009.
2. Warrier, A., et al., 2021, *Photodiagnosis and Photodynamic Therapy*. DOI: 10.1016/j.pdpdt.2020.102090
3. Kozlikova, M., et al., 2026, Journal of Medicinal Chemistry. DOI: 10.1021/acs.jmedchem.5c03090

POSTERS

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How to: Tin Corrole Photosensitisers

Bastian Kraul,[a] Johannes Zurwellen[b], Marla Brandtstäter[b], Anastasiia Riabchunova[b], Stefanie Tschierlei[b], Martin Bröring[a]

[a]*Institute of Inorganic and Analytical Chemistry, TU Braunschweig, Germany*
[b]*Institute of Physical and Theoretical Chemistry, TU Braunschweig, Germany*

Due to their electron-rich 18π system and trianionic character, corrole macrocycles can stabilize metals in high oxidation states from +3 to +6 [1]. This feature has been successfully used for numerous 3d and 4d transition metal complexes. On the other hand, main-group metal corroles [2, 3] are less common, and their redox behavior has been investigated only in a small number of antimony derivatives.
Tin corroles are redox-active and show great potential for catalysis [4]. They are reliable singlet oxygen photosensitisers [5] and are being tested for their activity in triplet-triplet annihilation photon upconversion. The poster will cover ongoing research and initial findings on the synthesis, characterisation, and (photo)reactivity of Sn(IV)-Corroles with various axial ligands.

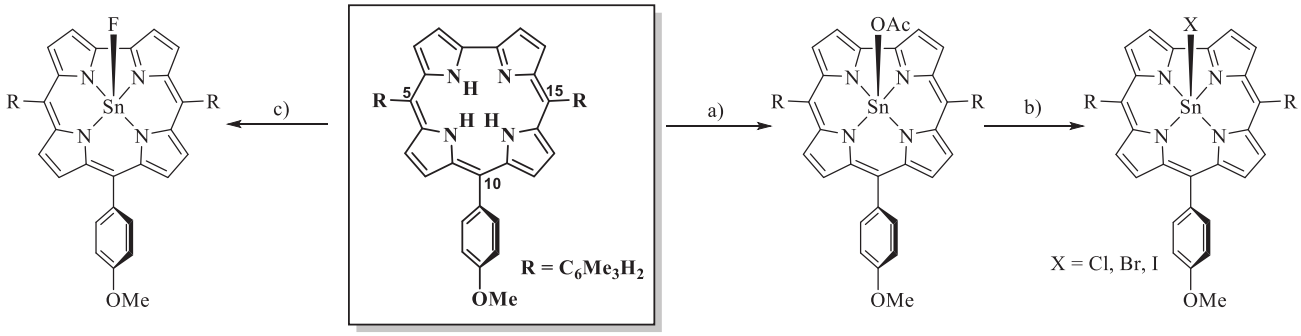


Figure 1. Preparation of tin(IV)corroles **SnOAcCor** and halogenated analogues **SnFCor**, **SnClCor**, **SnBrCor** and **SnICor**. a) $Sn(OAc)_2$, acetic acid, Δ; b) HCl/HBr/HI, CH_2Cl_2; c) SnF_2, dimethylformamide, Δ.

REFERENCES

[1] J. W. Buchler, M. J. Clarke, J. B. Goodenough, C. K. Jørgensen, D. M. P. Mingos, J. B. Neilands, G. A. Palmer, P. J. Sadler, R. Weiss, R. J. P. Williams et al., *Metal Complexes with Tetrapyrrole Ligands III*, Springer Berlin Heidelberg, Berlin, Heidelberg, **1995**.
[2] S. Eulberg, N. Schulze, J. Krumsieck, N. Klein, M. Bröring, *Angew. Chem. Int. Ed. Engl.* **2023**, *62*, e202306598.
[3] K. M. Kadish, D. Dubois, J. M. Barbe, R. Guilard, *Inorg. Chem.* **1991**, *30*, 4498–4501.
[4] W. Sinha, S. Kar, *Organometallics* **2014**, *33*, 6550–6556.
[5] V. Caliskanyürek, S. Eulberg, O. Lange, M. Bröring, S. Tschierlei, *Chem. Commun.* **2024**, *60*, 4096–4099.

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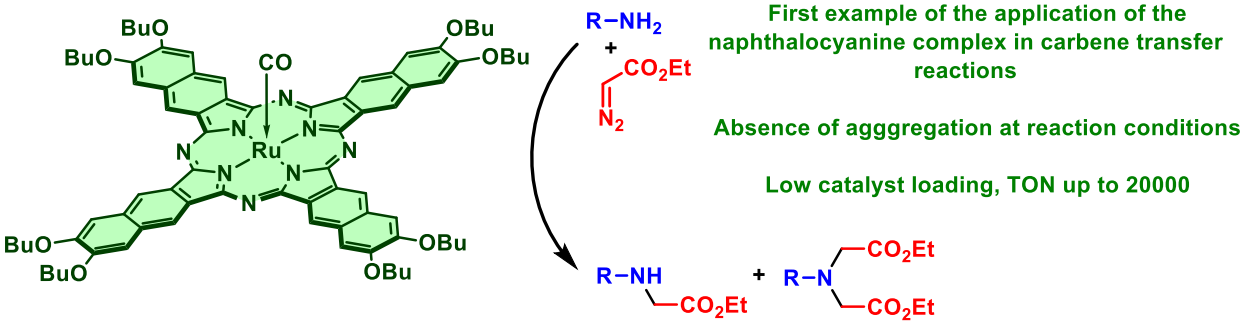
Ruthenium naphthalocyanine as catalyst of carbene insertion into N-H bonds.

Andrey P. Kroitor[a,c], Alexander G. Martynov[a], Yulia G. Gorbunova[a,b], Alexander B. Sorokin[c]

[a] *Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, 31-4 Leninsky Prospect, 119071 Moscow, Russia*
[b] *Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, 31 Lenisky Prospect, 119991 Moscow, Russia*
[c] *Institut de Recherches sur la Catalyse et l'Environnement de Lyon IRCELYON, UMR 5256, CNRS – Université Lyon 1, 2 av. A. Einstein, 69626 Villeurbanne, France*

Among carbene transfer reactions, which serve as useful tools for synthesizing various C – X functionalized compounds, carbene insertion into N – H bonds is considered challenging due to nitrogen's strong ability to coordinate to the metal center thus suppressing the catalytic activity. Ruthenium and iron complexes featuring porphyrin or phthalocyanine ligands have proven to be versatile catalysts for such transformations, achieving higher turnover numbers than traditional Rh-based catalysts. However, their expanded analogues – naphthalocyanine (Nc) complexes – have not previously been implemented in these reactions, likely due to low solubility and tendency to aggregation, which hinders reagent access to the metal center.

To tackle these issues, we recently synthesized ruthenium complex with octa-butoxy-napththalocyanine macrocycle. Due to the presence of an axial CO ligand this comples remained predominantly monomeric in the concentration range of 2–20 μM. This modified complex was investigated as a catalyst in the reactions between acceptor diazo compounds and various amines, achieving a turnover number (TON) of 20 000 – significantly surpassing the performance of previously studied ruthenium phthalocyanine catalysts [1].



Acknowledgement: this work was supported by the CNRS and RFBR through the International Emerging Action 2021 and the research project 21-53-15004 and by the Agence Nationale de Recherche (ANR), project ANR-23-CE07-0039.

REFERENCES

1. Kroitor AP et al. *Dalton Trans.* 2025; **54**: 4018-4024.

POSTERS

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Phospholipid Bicelles as Topical Delivery Systems for Porphyrinic Photosensitizers

Daja Krummenacher[a], Ilche Gjuroski[a], Peter Vermathen[b], Julien Furrer[a], Sabine Kässmeyer[c], Martina Vermathen[a]

[a]*University of Bern, Department of Chemistry, Biochemistry and Pharmaceutical Sciences, Bern, Switzerland*
[b]*University of Bern and Inselspital, Magnetic Resonance Methodology, Institute of Diagnostic and Interventional Neuroradiology, Bern, Switzerland*
[c]*University of Bern, Division of Veterinary Anatomy, Vetsuisse Faculty, Bern, Switzerland*

Topical photodynamic therapy (PDT) is a minimally invasive and safe treatment for various superficial skin diseases, such as actinic keratosis [1]. PDT treatment of skin employs the delivery of a precursor (5-ALA) that is converted into the active form, the photosensitizer (PS) protoporphyrin IX, followed by targeted irradiation. This causes the PS to undergo a photochemical reaction, producing reactive oxygen species, which induce oxidative damage to surrounding cells [2]. Directly applied porphyrinic PSs are promising candidates for topical PDT due to their absorbance within the therapeutic window [3]. However, these lipophilic compounds require solubilization to remain active for PDT; a carrier is necessary. Bicelles are biocompatible disc-shaped phospholipid nanocarriers. Their lipid bilayer offers an environment for lipophilic drug molecules [4]. Smaller than liposomes, bicelles might facilitate penetration into the skin surface. The aim of this current project is to investigate bicelles as a topical drug delivery system for porphyrinic PSs.

Bicelles with differently combined phospholipids were loaded with PSs (Chlorin e4, m-THPP, or m-THPC). During the bicelle production, the PSs were encapsulated. The resulting systems were characterized using NMR spectroscopy [5] and dynamic light scattering (DLS). With NMR spectroscopy, the formation of bicelles, drug encapsulation efficiency, and the size of the system could be determined. DLS was used to measure the size and stability of the empty bicelles. With the successful formulations, *in vitro* skin penetration tests were performed to investigate PS penetration into the skin, both by extracting the penetrated PS and by fluorescence microscopy of skin sections. Furthermore, cell uptake studies were conducted to quantify PS uptake in keratinocytes.

REFERENCES

1. Yang Y, Tu J, Yang D, Raymond JL, Roy RA, Zhang D, *Current Pharmaceutical Design*, **2019**, 25(4):401-412.
2. Abrahamse H, Hamblin MR, *The Biochemical Journal*, **2016**, 473(4), 347–364.
3. Castano AP, Demidova TN, Hamblin MR, *Photodiagnosis and Photodynamic Therapy*, **2004**, 1(4), 279–293.
4. Dufourc EJ, *Biochimica et Biophysica Acta. Biomembranes*, **2021**, 1863.
5. Gjuroski I, Furrer J, Vermathen M, *Molecules*, **2021**, 26 (2021) 1942.

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Additive-Controlled Polymorphism in a Chlorophyll-Based Supramolecular Polymer

Ryo Kudo[a], **Sho Takamiya**[a], **Hitoshi Tamiaki**[b], **Hiroki Hanayama**[c], **Shiki Yagai**[c,d]

[a]*Division of Advanced Science and Engineering, Graduate School of Science and Engineering, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan*
[b]*Graduate School of Life Sciences, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan*
[c]*Department of Applied Chemistry and Biotechnology, Graduate School of Engineering, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan*
[d]*Institute for Advanced Academic Research (IAAR), Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan*

In the light-harvesting antenna of purple photosynthetic bacteria, chlorophylls form circular mesoscale (*ca.* 10 nm) architectures using protein scaffolds, enabling highly efficient exciton diffusion [1]. To probe this structure–function relationship, self-assembly of synthetic chlorophyll derivatives has been explored. Although nanosheets or nanotubes have been constructed in the synthetic regime, there are few reports of self-assembled circular structures in the mesoscale [2]. Inspired by our scissor-shaped azobenzene dyads that self-assemble into uniform nanorings [3], we synthesized a scissor-shaped zinc chlorin **1** (Figure 1a) and investigated its self-assembly.

Upon aging a methylcyclohexane (MCH) solution of **1** prepared by a heating-cooling protocol for several days, AFM revealed elongated nanofibers with a minor fraction of uniform nanorings (*ca.* 14 nm) (Figure 1b). In the presence of 1-butanol, only nanofibers were obtained (Figure 1c), whereas the addition of pyridine resulted in the formation of nanorings as the major product (Figure 1d). A single *J*-type absorption band was visible at the Qy region with a bisignate CD band for the nanofiber solution, while the nanoring-rich solution exhibited two *J*-bands and corresponding two bisignate CD bands (Figure 1e), suggesting distinct stacking modes. The detailed mechanism of the self-assembly of **1** under different solvent conditions will be discussed.

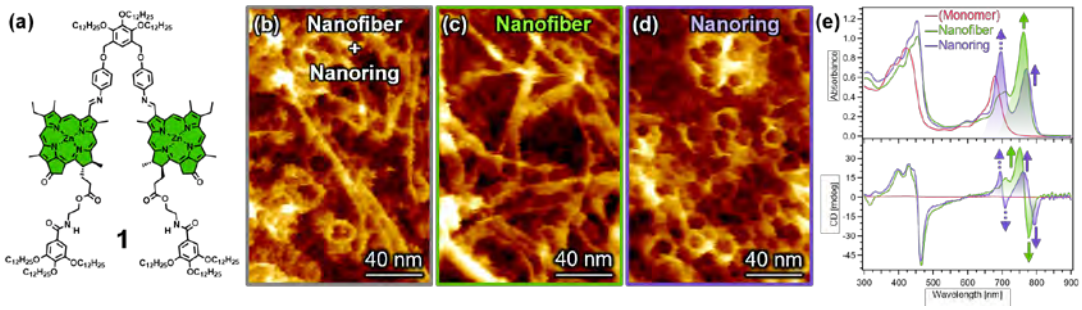


Figure 1. (a) Molecular structure of **1**. (b–d) AFM images of aggregates of **1** spin-coated from solutions in pure MCH (b), MCH containing 1-butanol (c), and MCH containing pyridine (d). (e) UV–Vis absorption (upper) and CD spectra (lower) of **1** in monomeric (red line), nanofiber-rich (green line), and nanoring-rich states (purple line).

REFERENCES

1. G. McDermott *et al.*, *Nature* **1995**, *374*, 517.
2. a) T. Ishii *et al.*, *Chem. Commun.* **2023**, *59*, 1967; b) R. Kudo *et al.*, *Org. Chem. Front.* **2024**, 11, 6304.
3. a) J. S. Valera *et al.*, *Angew. Chem. Int. Ed.* **2022**, *61*, e202114290; b) T. Saito *et al.*, *J. Am. Chem. Soc.* **2023**, *145*, 443.

POSTERS

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Modulated Vibronic Coupling in Deuterated Tetraaza[8]circulenes

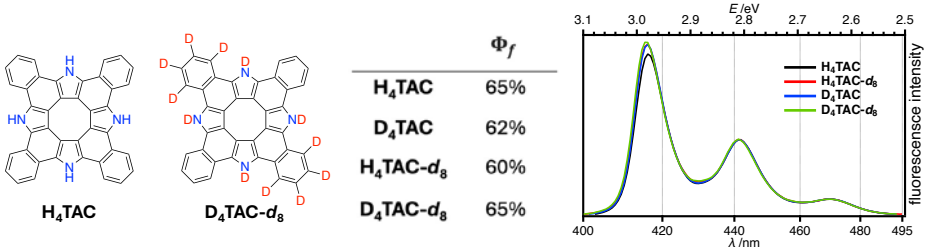
Yoh Kumagai[a], **Takayuki Tanaka**[a], **Shu Seki**[a]

[a] *Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Japan*

Vibronic coupling, the interaction between the electronic and vibrational states of a molecule, profoundly dictates photophysical properties, including intersystem crossing and non-radiative deactivation pathways. In the field of organic luminescent materials, the introduction of deuterium has been shown to alter specific molecular vibrational behaviors, leading to the modulation of non-radiative rate constants. While the enhancement of fluorescence quantum yields and photostability through selective deuteration has been reported in fluorescent molecules such as phthalocyanines[1], comprehensive studies that include the selective deuteration of highly symmetric molecules have remained limited. Such highly symmetric and rigid structural platforms are particularly desirable for theoretical analysis. Tetraaza[8]circulene (**H$_4$TAC**), a rigid π-conjugated molecule exhibiting 4-fold symmetry and blue fluorescence, displays well-structured vibronic bands in its absorption and emission spectra. Consequently, selectively deuterated **H$_4$TAC** provides an ideal model to systematically investigate the relationship between altered vibrational dynamics and photophysical characteristics.

To address the systematic understanding of the vibronic coupling, we first synthesized **H$_4$TAC** possessing deuterium at half of its peripheral hydrogen positions, *i.e.*, **H$_4$TAC-*d*$_8$**. This was achieved by substituting the conventional *ortho*-dibromobenzene with *ortho*-dichlorobenzene-d_4 in the established scheme[2]. Then, the NH protons of the framework were successfully exchanged for ND groups by the simple addition of D_2O to a THF solution, thereby affording **D$_4$TAC-*d*$_8$**. The successful isolation of **H$_4$TAC-*d*$_8$** was confirmed by the ^{1}H and ^{13}C NMR spectra and high-resolution mass spectrometry.

IR spectra further confirmed the structural modifications, where the sharp N-H stretching peak observed around 3440 cm^{-1} for **H$_4$TAC** and **H$_4$TAC-*d*$_8$** disappeared and was replaced by N-D stretching peaks around 2550 cm^{-1} in **D$_4$TAC** and **D$_4$TAC-*d*$_8$**. The fluorescence spectra of these selectively deuterated compounds, measured in dehydrated THF, did not exhibit any significant changes in their overall spectral configurations. However, the fluorescence quantum yields were shown to fluctuate upon deuteration, displaying Φ_f values of 65% for **H$_4$TAC**, 62% for **D$_4$TAC**, 60% for **H$_4$TAC-*d*$_8$**, and 65% for **D$_4$TAC-*d*$_8$**, after careful calibration of the self-absortpion process. By correlating our experimental results with theoretical calculations to provide a rigorous theoretical interpretation, we aim to systematically elucidate and control vibronic coupling through a combination of synthetic designs and theoretical models.



REFERENCES

1. N. Toriumi, A. Muranaka, M. Uchiyama, *Chem. Pharm. Bull.* **2023**, *71*, 459.
2. F. Chen, Y. S. Hong, S. Shimizu, D. Kim, T. Tanaka, A. Osuka, *Angew. Chem. Int. Ed.* **2015**, *54*, 10639.

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POSTERS



Photo-assisted Organic Transformations by Palladium Dipyrrinato Complexes

Shekhar Kumar[a], Samrita Sharma[a], Iti Gupta[a]

[a]*Department of Chemistry, Indian Institute of Technology, Gandhinagar,382055, Gujarat, India*

Photocatalysis has emerged as a greener and sustainable approach for organic transformation.[1-2] In recent years, metal dipyrrinato complexes have shown promise in the photoxidation of organic compounds.[3] Metal dipyrrinato complexes acquire high absorption coefficients in the visible region.[4] Heavy atom effect in dipyrrinato complexes leads to the formation of long-lived triplet excited states. Also, these complexes exhibit excellent singlet oxygen generation quantum yields.[5] These properties make them promising photocatalysts for various photochemical oxidative transformations.

In this poster, we have synthesized a series of homo-leptic and hetero-leptic Pd(II)dipyrrinato complexes and utilized them for efficient photocatalytic oxidative cleavage of indole derivatives. The oxidative coupling between benzaldehyde and amine, also explored with Pd(II)-dipyrrinato complex. We also demostrated a method for the functionalization of 1,2,3,4-tetrahydroisoquinoline derivatives using Pd(II)-dipyrrinato complex as catalyst. These methods demonstrated functional group tolerance and provided an effective strategy for synthesizing a diverse range of products in a highly efficient manner, validating the versatility of Pd(II)dipyrrinato complexes as photocatalysts for various organic transformations. Notably, these photochemical transformations require only a minimal catalyst loading of 0.05 mol% for these reactions, demonstrating their exceptional cost-effectiveness.

POSTERS

REFERENCES

1. Prier, C. K.; Rankic D. A.; Macmillan D. W. C. Chem. *Rev.* **2013,** *113*, 5322-5363.

2. Skubi, K. L.; Blum, T. R.; Yoon, T. P. *Chem. Rev.* **2016**, *116*, 17, 10035–10074

3. Manav N.; Singh, R.; Janaagal, A.; Yadav, A. S.; Pandey, V. and Gupta, I., *New J. Chem*, **2022,** 40, 19310-19321.

4. Kumar, S.; Agarwal, K.; Sanyam, Mondal, A. and Gupta, I., *Chem.: Asian. J.* **2024,** e202400680.

5. Manav N. ; Lone, M. Y. ; Raza, M. K. ; Chavda, Mori, J. S. and Gupta, I., *Dalton Trans*. **2022**, 51, 3849-3863.

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NMR Detection of Enantiomeric Excess w/o Formation of Diastereomers using Prochiral Solvating Agents (*pro*-CSAs)

Jan Labuta, Shinsuke Ishihara, Jonathan P. Hill

Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Tsukuba, Japan (Labuta.Jan@nims.go.jp)

Chirality is a key feature in many biological events. The two enantiomers of the same molecule act differently when interacting with other chiral species. It is essential in the development of new pharmaceuticals, where the pharmacological effect depends on the identity of the enantiomer (e.g., ibuprofen, atropine, thalidomide, etc.). Versatile ^{1}H NMR prochiral solvating agents [1-8] (*pro*-CSAs, see an example of prochiral host **H** in Fig.1a) for the determination of enantiomeric excess (*ee*) are presented. The sensing mechanism doesn't rely on the formation of diastereomeric pairs between the prochiral host and chiral analyte (e.g., ibuprofen); instead, a pair of enantiomeric complexes is formed (Fig.1b,c) [1-8]. The *pro*-CSA host molecule contains prochiral CH reporter groups (e.g., pyrrolic β-protons, Fig.1a), which facilitate *ee* discrimination. The model of the sensing mechanism exhibits a linear response between *ee* of the analyte and the observed magnitude of induced chemical shift non-equivalence ($\Delta\delta$) in the ^{1}H NMR spectra of the host **H** (Fig.1d,e). The effect is demonstrated for various chiral analytes, including carboxylic acids and esters, amino acid esters, N-protected amino acids, and some terpenoids.

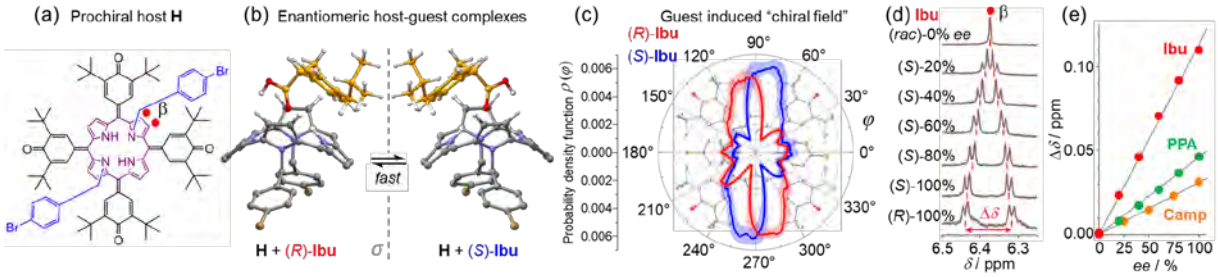


Fig.1. (a) Structure of prochiral porphyrin derivative **H**. (b) Schematic illustration of the enantiomeric complexes. (c) Molecular dynamics simulation of the sensing mechanism. (d) NMR spectra of porphyrin β-H reporting group in the presence of various *ee* of ibuprofen (**Ibu**) analyte. (e) Fundamental linear relationship between induced chemical shift non-equivalency $\Delta\delta$ and *ee* as obtained from ibuprofen (**Ibu**), 2-phenoxypropionic acid methyl ester (**PPA**), and camphor (**Camp**).

REFERENCES

1. A. Shundo, J. Labuta, J. P. Hill, S. Ishihara, and K. Ariga. *J. Am. Chem. Soc.* **2009**, *131*, 9494.
2. J. Labuta, S. Ishihara, A. Shundo, S. Arai, S. Takeoka, K. Ariga, and J. P. Hill. *Chem. Eur. J.* **2011**, *17*, 3558.
3 J. Labuta, S. Ishihara, T. Šikorský, Z. Futera, A. Shundo, L. Hanyková, J. V. Burda, K. Ariga, and J. P. Hill. *Nat. Commun.* **2013**, *4*, 2188.
4. J. Labuta, J. P. Hill, S. Ishihara, L. Hanyková, K. Ariga. *Acc. Chem. Res.* **2015**, *48*, 521**.**
5. J. Labuta, S. Ishihara, J. P. Hill. *J. Porphyrins Phthalocyanines* **2020**, *24*, 320.
6. M. K. Chahal, N. Velychkivska, W. A. Webre, J. Labuta, S. Ishihara, K. Ariga, F. D'Souza, J. P. Hill. *J. Porphyrins Phthalocyanines* **2019**, *23*, 1184.
7. S. Ishihara, J. Labuta, Z. Futera, S. Mori, H. Sato, K. Ariga, J. P. Hill. *J. Phys. Chem. B* **2018**, *122*, 5114.
8. K. Takimoto, S. Ishihara, J. Labuta, V. Březina, D. T. Payne, J. P. Hill, K. Ariga, M. Sumita, S. Mori, H. Sato. *J. Phys. Chem. Lett.* **2020**, *11*, 8164.

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Phase-Separable and pH-Sensitive Star-Shaped Porphyrin-PNIPAM Conjugates

Jan Labuta, Nadiia Velychkivska

Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Tsukuba, Japan (Labuta.Jan@nims.go.jp)

Star-shaped porphyrin-PNIPAM (**PP**) conjugates with four PNIPAM arms connected to a central porphyrin unit were synthesized using RAFT polymerization [1] (Fig.1a). Temperature-induced phase separation (Fig.1b,c) behaviour of **PP** was investigated and analyzed by a two-state phase separation model [2,3]. The LCST (type II) phase diagram was constructed using Flory−Huggins theory. Below the phase-separation temperature (T_p), **PP** behaves as a 1D supramolecular polymer with a concentration-dependent length, while above T_p, **PP** adopts larger spherical globular structures (Fig.1b). Various temperature−pH reversible and irreversible interdependencies ("cross-effects") between phase separation and protonation were observed by NMR, DSC, SAXS, DLS, and UV-Vis [1].

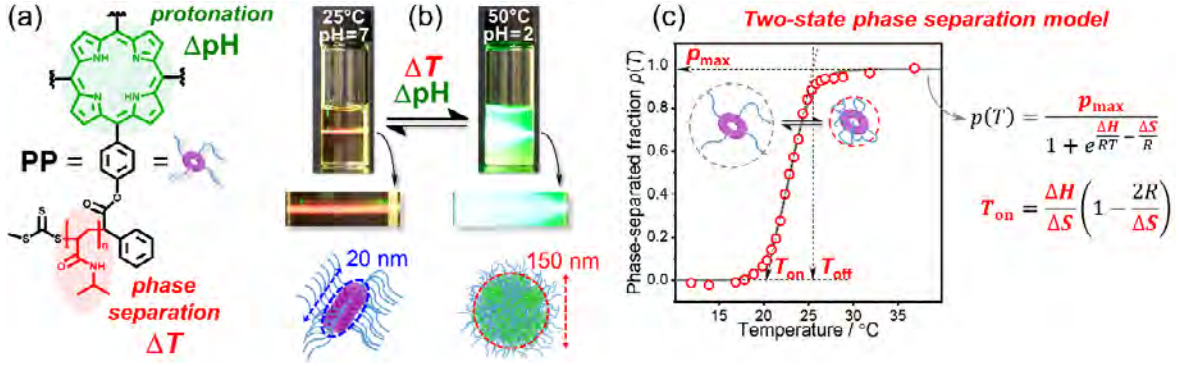


Fig. 1. (a) Structure of **PP** (only one arm is shown) [1]. (b) Illustration of temperature (ΔT) or pH (ΔpH) change on an aqueous solution of **PP**. Vials are irradiated with a green laser pointer (532 nm). (c) Two-state model of phase separation [2,3] fitted to NMR data.

REFERENCES

1. "Phase separation and pH-dependent behavior of 4-arm star-shaped porphyrin-PNIPAM$_4$ conjugates", Velychkivska N., Sedláček O., Shatan A. B., Spasovová M., Filippov S. K., Chahal M. K., Janisova L., Brus J., Hanyková L., Hill J. P., Winnik F. M., Labuta J., Macromolecules 55, 2109−2122 (2022).
2. "Improving the Colloidal Stability of Temperature-Sensitive Poly(*N*-isopropylacrylamide) Solutions Using Low Molecular Weight Hydrophobic Additives", Velychkivska, N., Starovoytova, L., Březina, V., Hanyková, L., Hill, J. P., Labuta, J., ACS Omega 3, 11865−11873 (2018).
3. "Thermodynamic and kinetic analysis of phase separation of temperature-sensitive poly(vinyl methyl ether) in the presence of hydrophobic *tert*-butyl alcohol", Velychkivska, N., Bogomolova, A., Filippov, S. K., Starovoytova, L., Labuta, J., Colloid Polym. Sci. 295, 1419−1428 (2017).

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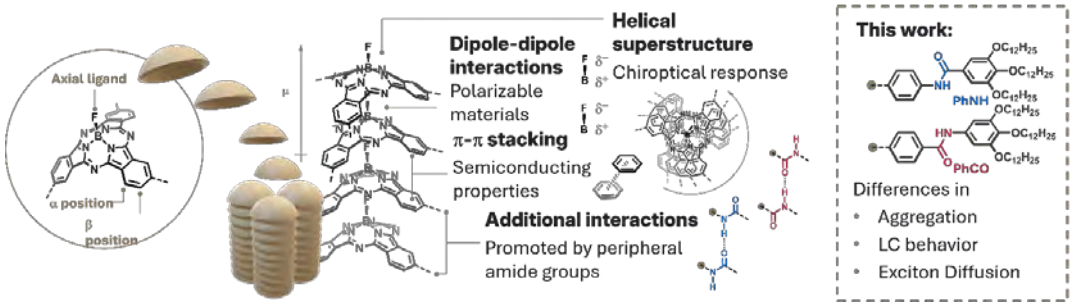


Driven by Geometry: Subphthalocyanines in Supramolecular Polymer Design

Juan Laforga-Martín[a], **Jorge Labella**[a,b], **Tomás Torres**[a,c,d]

[a]*Department of Organic Chemistry, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain.*
[b]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan.*
[c]*IMDEA-Nanociencia, c/Faraday 9, Cantoblanco, 28049 Madrid, Spain.*
[d]*Institute for Advanced Research in Chemical Sciences (IAdChem), 28049 Madrid, Spain.*

Molecular materials, based on the controlled organization of discrete molecules through non-covalent interactions, offer a versatile platform for developing functional systems with tailored properties. Among them, Subphthalocyanines (SubPcs) stand out as promising molecular building blocks for supramolecular polymers due to their non-planar geometry, intrinsic dipole moment, and ability to assemble into (chiral) columnar structures.[1] These stacked architectures are particularly appealing for organic electronics, as the resulting molecular polarization along the columns may give rise to directional charge transport. In order to achieve such columnar assemblies, SubPcs require specific structural features: a non-bulky axial group —typically fluorine— to favor π–π stacking, and peripheral amide groups to promote directional hydrogen bonding.[2] In this work, we investigate how subtle modifications in the amide connectivity influence the supramolecular organization and functional properties of SubPc-based systems. Two series of trisubstituted SubPcs, bearing amides connected via either PhNH or PhCO moieties, were synthesized and their self-assembly behavior in solution was comprehensively studied. Moreover, their liquid-crystalline (LC) phases and exciton diffusion capabilities were evaluated. Our results reveal this minor variation in the amide-to-core connectivity dramatically impacts the aggregation thermodynamics, liquid-crystalline behavior, and exciton diffusion properties, underscoring the importance of precise supramolecular engineering in the design of functional molecular materials.



REFERENCES

1. Lavarda, G. et al.; *Chem. Soc. Rev.* **2022**, 51, 9482-9619.
2. Mayoral, M. J. et al.; *J. Am. Chem. Soc.* **2020**, 142, 21017.

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Combining Pyrrole Chemistry with Solid-phase Peptide Synthesis: Modular Approaches for Peptide Multifunctionalization

Pak-Lun Lam[a], Ho-Fai Chau[a], Wing-Sze Tam[a,b], Waygen Thor [a], Yik-Hoi Yeung[a], Hei-Yui Kai[a], Yue Wu[a], Ka-Leung Wong[c]

[a] *Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong SAR*
[b] *Department of Chemistry, Hong Kong Baptist University, 224 Waterloo Rd, Kowloon Tong, Kowloon, Hong Kong SAR, China.*
[c] *Department of Chemistry, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong SAR, China. Email: klwong@cityu.edu.hk* (Prof. K.-L. Wong)

Pyrrole chemistries refer to the reactions to synthesize a variety of functional moieties like dipyrrins/BODIPYs, porphyrins, and corroles. Solid-phase peptide synthesis (SPPS) is a modular approach to synthesizing peptide derivatives in both laboratories and industries. Previously, to synthesize peptide derivatives that bear the above-mentioned functional moieties, additional synthetic steps are inevitable to prepare the corresponding building blocks, followed by conjugating to peptides. In our studies, by strategically combining the pyrrole chemistries with SPPS, we established a series of synthetic methodologies to modularly construct these functional moieties on peptides. With our approaches, the chemists can obtain these functional peptides more quickly, and the products are easier to diversify in the late stage. Moreover, the products from our synthetic approach also display a wide range of applications as theragnostic agents and biocompatible materials.

REFERENCES

1. *Chem. Sci.* **2020**, *11*, 11266–11273.
2. *Angew. Chem. Int. Ed.* **2021**, *60*, 20301–20307.
3. *Angew. Chem. Int. Ed.* **2022**, *61*, e202207532.
4. *Chem. - A Eur. J.* **2023**, *29*, e202203623.
5. *Adv. Sci.*, **2025**, *12*, 2409771.

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Tunable Photodynamic Efficiency in Porphyrin Nanoparticles via Polymorphsm-like Molecular Packing

Hosoowi lee[a], Juyong Yoon[a]

[a]*Department of Chemistry & Nanoscience, Ewha Womans University, Korea*

Photodynamic therapy (PDT) is fundamentally governed by the photophysical properties of photosensitizers, which are highly sensitive to molecular aggregation. While aggregation-caused quenching (ACQ) has been extensively studied in solution-phase systems, the influence of solid-state molecular packing on photodynamic performance remains largely unexplored. In other material domains, including pharmaceuticals and inorganic systems, polymorphism is known to critically affect functional properties, suggesting that similar effects may exist in PDT-relevant organic assemblies.

Here, we report a porphyrin-based photosensitizer rationally designed with sterically bulky substituents to suppress ACQ. Unlike conventional porphyrins that typically form amorphous aggregates during nanoparticle fabrication, this molecule undergoes ordered self-assembly, as revealed by GI-WAXS analysis. Importantly, variations in purification conditions lead to distinct stacking arrangements, exhibiting polymorphism-like behavior in the solid state.

We found that these differences in molecular packing significantly influence the self-assembly pathway during nanoparticle formation in aqueous environments. As a result, nanoparticles derived from different packing states exhibit markedly different ROS generation efficiencies.

These findings demonstrate that the solid-state organization of organic photosensitizers can serve as a critical determinant of photodynamic activity. Controlling polymorphism-like molecular packing thus offers a new structural design principle for enhancing PDT performance.

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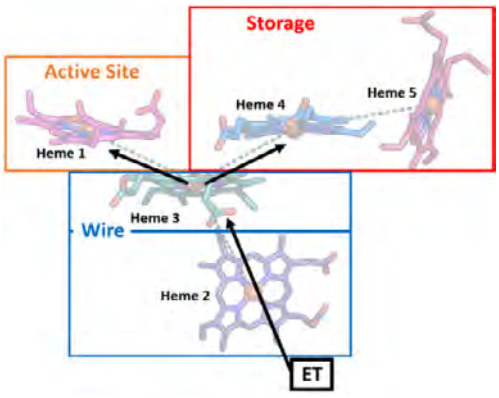
Trapping and Spectroscopic Characterization of the Ferrous Heme-NO Intermediate of Bacterial Multiheme Cytochrome c Nitrite Reductase

Cybele Lemuh Njimoh[a], Krystina Hird[b], Eric L. Hegg[b], Nicolai Lehnert[a]*

[a]*Department of Chemistry, The University of Michigan, Ann Arbor, Michigan 48109, United States*
[b]*Department of Biochemistry & Molecular Biology, Michigan State University, East Lansing, Michigan 48824, USA*

Multielectron biological redox reactions and the metalloenzymes that catalyze them are critical in various metabolic processes, including O_2 evolution, aerobic and anaerobic respiration, N_2 fixation, and nitrogen assimilation. One particularly important enzyme in the global nitrogen cycle is the pentaheme Cytochrome *c* nitrite reductase (NrfA). NrfA catalyzes the remarkable six-electron and eight-proton reduction of nitrite (NO_2^-) to ammonium (NH_4^+), the key step in anaerobic nitrate (NO_3^-) respiration in the **D**issimilatory **N**itrate **R**eduction to **A**mmonium (DNRA) pathway.[1] Several crystal structures are available for NrfA from different model organisms. Our work focuses on NrfA from *Geobacter lovley*, an environmentally relevant bacterium. Consistent with all NrfA structures reported to date, *G. lovleyi* NrfA crystallizes as a homodimer with each subunit containing five *c*-type hemes covalently linked to the protein backbone.[2] Four of the hemes (Hemes **2** - **5**) exhibit bis-His coordination and are used to store and/or transfer electrons, whereas the Lys-coordinated Heme **1** constitutes the active site of the enzyme.

To understand how the pentaheme scaffold of NrfA is charged with electrons, we first determined how to reduce the hemes of NrfA in clean one-electron steps and monitored heme reduction by EPR spectroscopy. Combined with spectral simulations, this allowed us to assign the complex EPR spectra of NrfA, determine the sequence in which the hemes are reduced, and assign reduction potentials to all hemes. These results show that Hemes **2** and **3** provide an electron transfer pathway, Hemes **4** and **5** serve as an electron storage unit, and Heme **3** is the central electron distributor (see right).[3] We further interrogated the NO intermediates of the catalytic cycle of NrfA using EPR and resonance Raman spectroscopy, as well as suitable enzyme variants.



Electron transfer within NrfA. Heme **2** and Heme **3** act as a wire, and Heme **3** distributes the electrons to the storage Hemes **4** and **5** or the active site Heme **1**.

REFERENCES

1. K. Hird, J. O. Campeciño, N. Lehnert, E. L. Hegg, *J. Inorg. Biochem.* 2024, 247, 112542.
2. J. Campeciño, S. Lagishetty, Z. Wawrzak, V. Sosa Alfaro, N. Lehnert, G. Reguera, J. Hu, E. Hegg, *J. Biol. Chem.* 2020, 295, 11455-11465. Erratum: J. Biol. Chem. 2022, 298, 102743
3. V. Sosa Alfaro, J. Campeciño, M. Tracy, S. J. Elliott, E. L. Hegg, N. Lehnert, *Biochemistry* 2021, 60, 1853-1867.

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Lessard Research Group: Electronics and Sensors Based on Phthalocyanines and Beyond

Benoît H. Lessard[a,b]

[a]*Department of Chemical and Biological Engineering, University of Ottawa, 161 Louis Pasteur, Ottawa, Ontario K1N 6N5, Canada.*
[b]*School of Electrical Engineering and Computer Science, University of Ottawa, 800 King Edward Ave. Ottawa, Ontario K1N 6N5, Canada.*



The Lessard Research Group (LRG) at the University of Ottawa is committed to pioneering low-cost, sustainable electronic technologies through interdisciplinary research that bridges materials chemistry, device engineering, and applied data science. Our work focuses on the molecular design, synthesis, and integration of novel carbon-based materials into next-generation organic electronic and photonic systems, including printed sensors, organic thin-film transistors (OTFTs), and flexible electronic prototypes.

We explore fundamental structure–property relationships to optimize performance[1,2] and stability[3], while also prioritizing scalable, recyclable, and green materials[4] that align with sustainable manufacturing and end-of-life considerations. Our research spans sensors for chemical and biological targets, innovative polymeric dielectrics and semiconductors, and automated approaches[5,6] to accelerate materials discovery and device fabrication.

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Come learn what we can do and how we can collaborate together!

REFERENCES

1. Advanced Functional Materials, 2024, 2408779
2. Advanced Functional Materials, 2025, e14609
3. Small Science, 2025, e202500452
4. ACS Applied Materials & Interfaces, 2025, 17, 1734-1742
5. Advanced Electronic Materials, 2025, 2400500
6. Small Methods, 2025, e00782

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Spectroscopic Properties of Chiral Porphyrin Self-Assembled Monolayers on Thin Ferromagnetic Films

A.Lewandowska-Andralojc[a], K. Hauza[a,b], G. Burdzinski[c], A. Lindner[d], J. Lindner[d], R. Salikhov[d], B. Marciniak[a,b]

[a]*Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznanskiego 8, 61-614 Poznan, Poland*
[b]*Center for Advanced Technologies, AMU, Uniwersytetu Poznanskiego 10, 61-614 Poznan, Poland*
[c]*Faculty of Physics, AMU, Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*
[d]*Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany*

In recent years, the so-called *spinterface*—the interface between ferromagnetic and molecular materials—has gained considerable attention as an ideal platform for generating new spin-related effects. [1] Even though molecular spintronics, where the *spinterface* plays a central role, is a vividly developing field, surprisingly little has been done to explore the potential of inorganic/organic interfaces in combination with the advantages offered by light-induced processes in organic chromophores. [2]
Porphyrin chromophores were covalently anchored to thin gold-capped ferromagnetic films (FM/Au) through chiral oligopeptide chains, forming a self-assembled monolayer (SAM) (Fig. 1). The properties of such FM/Au/SAM inorganic/organic interfaces were studied in parallel via (***i***) photochemical methods (*steady-state and transient absorption spectroscopy*) allowing detailed characterization of the behavior of the photoexcited molecular layer in the proximity of the FM, and (***ii***) *ferromagnetic resonance spectroscopy* (FMR), being an exceptionally sensitive method for detecting changes in the magnetic properties of the FM, here induced by the molecules in their ground and photoexcited states.

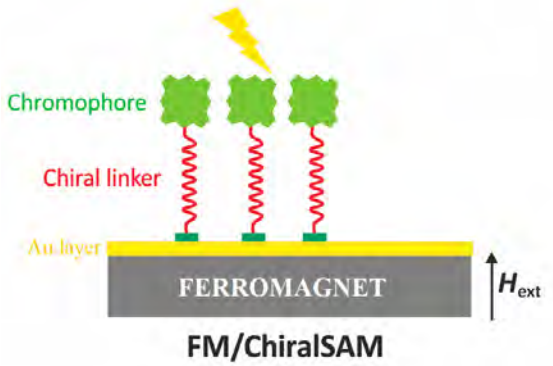


Fig. 1 Schematic representation of FM/chiral self-assembled monolayer system.

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REFERENCES

1. M. Cinchetti *et al.*, *Nat. Mater.* 16 (2017) 507.
2. J. M. Abendroth *et al.*, *ACS Nano* 13 (2019) 4928.

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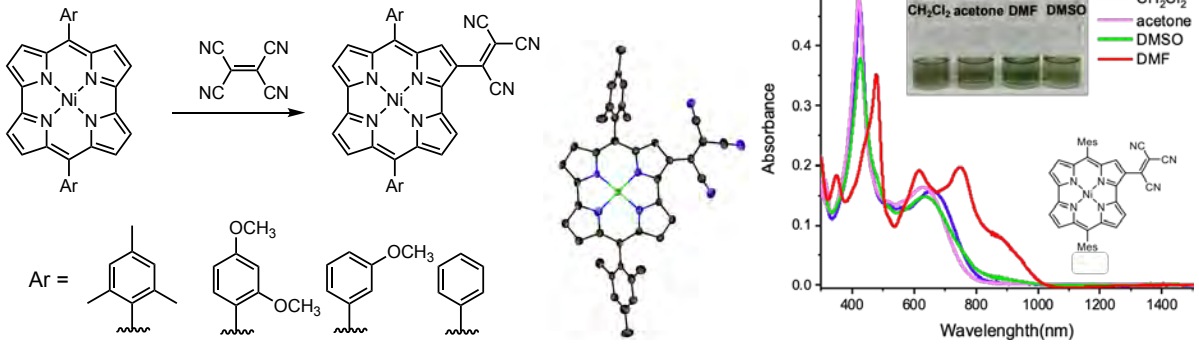


The reaction of Ni(II) norcorroles with TCNE

Sha Li[a], Qizhao Li[a], Shusaku Ukai[a], Hideaki Takano[a], Hiroshi Shinokubo[a]

[a]*Department of Molecular and Macromolecular Chemistry, Graduate School of Engineering, Nagoya University, Chikusa-ku, Nagoya 464-8603, Japan*

Norcorrole is a ring-contracted porphyrinoid that shows distinct antiaromaticity.[1] Antiaromatic norcorroles provide a promising platform for intramolecular charge transfer complexes due to their high HOMO and low LUMO energy levels as well as their unique redox properties.[2] In this study, we found that the treatment of Ni(II) diarylnorcorroles with tetracyanoethylene (TCNE) resulted in the formation of the addition products through regioselective C–C bond formation. Norcorroles with electron-donating substituents, such as dimesitylnorcorrole and 2,4-dimethoxyphenylnorcorrole, afforded the corresponding double addition products. The structure of the adduct obtained from dimesitylnorcorrole was clearly revealed by the X-ray diffraction analysis. Electrochemical analysis of the adduct exhibited anodic shifts in both the first oxidation and the first reduction processes relative to the parent norcorrole. The absorption spectra of the adduct displayed clear solvent-dependent features in the near-infrared (NIR) region.



REFERENCES

1. Ito, T.; Hayashi, Y.; Shimizu, S.; Shin, J.-Y.; Kobayashi, N.; Shinokubo, H. *Angew. Chem. Int. Ed.* **2012**, *51*, 8542.
2. Shin, J.-Y.; Yamada, T.; Yoshikawa, H.; Awaga, K.; Shinokubo, H. *Angew. Chem. Int. Ed.* **2014**, *53*, 3096.

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Chlorination of N-confused porphyrin

Angelina Liu[a], **Runchang Liu**[b]

[a] *Seaquam Secondary School (Canada)*
[b] *University of British Columbia*

DDQ (2,3-dichloro-5,6-dicyano-1,4-benzoquinone) is commonly employed as a strong oxidant and has also been shown to function as a chlorinating agent for aromatic substrates with notable regioselectivity.[1] In this work, we demonstrate that DDQ can be utilized as an efficient chlorinating agent for the selective chlorination of an *N*-confused porphyrin.

Halogenation of *N*-confused tetraphenylporphyrin (NCTPP) using conventional reagents such as *N*-bromosuccinimide (NBS) or *N*-chlorosuccinimide (NCS) is known to induce skeletal rearrangement, leading to the formation of *N*-fused porphyrins (NFPs), a distinct class of porphyrinoids characterized by an inner tri-pentacyclic ring system.[2]

In contrast, we report that under basic conditions, DDQ selectively chlorinates free base *N*-confused porphyrins at the C21 position, with the chlorine atom oriented toward the inner cavity of the *N*-confused macrocycle. The chlorinated N-confused porphyrin is confirmed by single-crystal X-ray diffraction analysis. This chlorination mode provides a tunable platform for modulating the electronic properties of *N*-confused porphyrins compared to their non-chlorinated counterparts. Density functional theory (DFT) calculations were performed to rationalize the observed regioselectivity of the chlorination process.

Meanwhile, we observed that DDQ itself undergoes a rearrangement under basic conditions. This rearranged DDQ species was unambiguously identified and confirmed by single-crystal X-ray diffraction analysis.

REFERENCES

1.Zhang, Q.; Yang, F.; Wu, Y. DDQ: the chlorinating reagent and oxidant for the ligand-directed ortho-chlorination of 2-arylpyridines. Org. Chem. Front. 2014, 1, 694–697. https://doi.org/10.1039/C4QO00076E
2. Furuta, H.; Ishizuka, T.; Osuka, A.; Ogawa, T. 'N-Fused Porphyrin' from N-Confused Porphyrin. J. Am. Chem. Soc. 1999, 121 (12), 2945–2946. https://doi.org/10.1021/ja9902672

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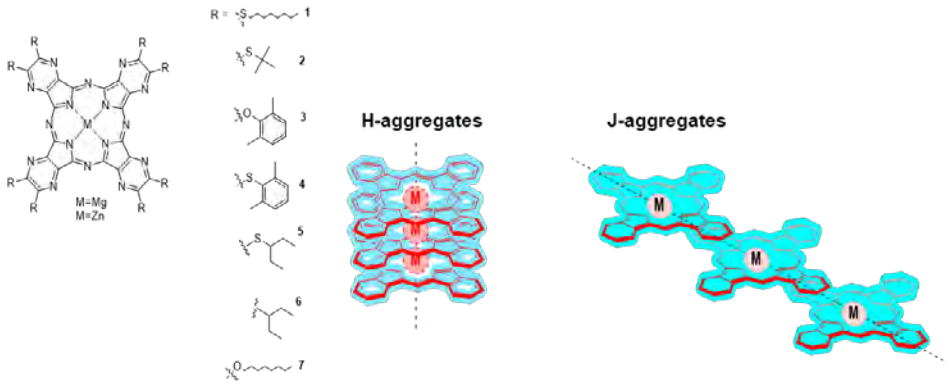


Self-assembled fluorescent J-dimers of phthalocyanines

Khaoula Lmcharrag [a], Stefan Bednarik [a], Veronika Novakova [a], Petr Zimcik [a]

[a] *Department of Pharmaceutical Chemistry and Pharmaceutical Analysis, Faculty of Pharmacy in Hradec Králové, Charles University, Akademika Heyrovskeho 1203, Hradec Králové 50003 e-mail:lamchark@faf.cuni.cz*

Phthalocyanines (Pcs) and their Aza-analogues (AzaPcs) are synthetic macrocyclic dyes composed of four isoindoline units connected by azomethine bridges [1,2]. Upon the discovery of Pcs, significant interest was generated to them due to their applications [3], as dyes and pigments, in optoelectronics, as photosensitizers in photodynamic therapy, where light absorption in far-red or near-infrared region above 680 nm triggers the release of reactive oxygen species. The properties mentioned above are typically related to the monomolecular state of the molecules. The planar Pc core tends to form H-type aggregates in vast majority of cases that are characterized by the eliminated fluorescence emission and the increase in absorption at blue shifted wavelengths. However, in specific situations upon proper design, atypical and extremely rare, slipped J-dimers are formed, unlike H-dimers, they exhibit red shifted absorption band and retained fluorescence (unless it is quenched by other photophysical processes). This project focuses on the synthesis of fluorescent J-dimers which will include synthesis of precursors, followed by cyclotetramerization, photophysical and spectral evaluation of prepared macrocycles.



Schematic representation of the target AzaPcs that are forming J-dimers

This work was supported by Charles University Grant Agency (GAUK 414725).

REFERENCES

1. 1. de la Torre, G.; Claessens, C. G.; Torres, T. Phthalocyanines: old dyes, new materials. Putting color in nanotechnology Chem. Commun. 2007, 2000-2015.
2. Novakova, V.; Donzello, M. P.; Ercolani, C.; Zimcik, P.; Stuzhin, P. A. Tetrapyrazinoporphyrazines and their metal derivatives. Part II: Electronic structure, electrochemical, spectral, photophysical and other application related properties Coord. Chem. Rev. 2018, 361, 1-73.
3.Wohrle, D.; Schnurpfeil, G.; Makarov, S. G.; Kazarin, A.; Suvorova, O. N. Practical Applications of Phthalocyanines – from Dyes and Pigments to Materials for Optical, Electronic and Photo-electronic Devices Macroheterocycles 2012, 5, 191-202.

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Photo-caged β-Lapachone Prodrugs

Ivonne R. Lopez-Miranda[a,b], **Andrew A. Beharry**[a,b]

[a]*Department of Chemical and Physical Sciences, University of Toronto Mississauga, Mississauga, Ontario L5L 1C6, Canada*
[b]*Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6, Canada*

β-lapachone is a natural product quinone that has potent anti-cancer activity for pancreatic, prostate, breast, and lung cancer. Its anticancer activity is dependent on the intratumoural activity of an overexpressed enzyme, NAD(P)H quinone oxidoreductase 1 (NQO1), which mediates the two-electron reduction of ß-lapachone to its unstable hydroquinone form that spontaneously re-oxidizes, completing a futile redox cycle producing cytotoxic reactive oxygen species (ROS) in the process [1]. ROS disrupts cell integrity, affecting pathways relating to cancer cell growth, leading to cell death [1]. Cancer cells express more NQO1 than healthy tissues, so ß-lapachone can be selectively toxic to cancer cells. However, ß-lapachone causes methemoglobinemia (oxidation of iron in red blood cells) and has poor pharmacokinetics with a half-life of 20 minutes [2]. We found that β-lapachone modified with a photolabile protecting group (7-diethylaminocoumarin) improved its stability in blood and reduced the formation of methemoglobinemia [3]. Irradiation using 420 nm light released the active β-lapachone, which effectively killed cancer cells.

With the goal of synthesizing a more potent photoactivatable β-lapachone, we caged β-lapachone with a novel photosensitizer, 3-bromo-7-diethylaminocoumarin, to investigate the synergistic effects of releasing β-lapachone while generating additional reactive oxygen species from the released photosensitizer. In vitro (^{1}H NMR, HPLC, UV-vis) studies confirmed the lack of NQO1 activity in the dark and rapid restoration of native β-lapachone upon irradiation, resulting in NQO1 activity. Higher ROS production was observed in irradiated samples, not in those kept in the dark. Critically, the amount of ROS produced was substantially higher than that observed with our original non-brominated photocaged β-lapachone, consistent with our design for both enzyme- and light-driven ROS production.

To test our brominated photocaged β-lapachone in cells, we selected U251 and T98G, two glioblastoma lines with poor native ß-lapachone response despite high NQO1 expression [4]. We observed the highest potency (EC_{50} = 320 ±40 nM) when cells were irradiated at 420 nm, compared with dark controls. We hypothesize that our prodrug exhibits higher cell permeability than native ß-lapachone and, together with light-mediated ROS production, results in higher potency than our original prodrug. Co-administration of our photocaged prodrug with the NQO1 inhibitor dicumarol demonstrated even greater potency (EC_{50} = 40 9 nM), which we attribute to ferroptosis activation. We hypothesize that inhibition of NQO1 by dicumarol allows ß-lapachone to inhibit the thioredoxin system, leading to overwhelming cancer cell death. Lastly, while the prodrug still absorbs 420 nm light, we discovered that this compound was also two-photon-activatable, absorbing at 900 nm and deeply penetrating tissues.

REFERENCES

1. Gong, Q.; Hu, J.; Wang, P.; Li, X.; Zhang, X. A Comprehensive Review on β-Lapachone: Mechanisms, Structural Modifications, and Therapeutic Potentials. *Eur. J. Med. Chem.* **2021**, *210*, 112962. https://doi.org/10.1016/j.ejmech.2020.112962.
2. Ma, X. et al. Esterase-activatable β-lapachone prodrug micelles for NQO1-targeted lung cancer therapy. J. Control. Release 200, 201–211 (2015).
3. Kaye, E. G.; Mirabi, B.; Lopez-Miranda, I. R.; Dissanayake, K. C.; Banerjee, U.; Austin, M.; Lautens, M.; Winter, A. H.; Beharry, A. A. Photo-Uncaging by C(Sp3)–C(Sp3) Bond Cleavage Restores β-Lapachone Activity. J. Am. Chem. Soc. 2023, 145 (23), 12518–12531. https://doi.org/10.1021/jacs.3c00398.
4. Zheng, L. et al. NQO1 drives glioblastoma cell aggressiveness through EMT induction via the PI3K/Akt/mTOR/Snail pathway. Int J Oncol 63, 110 (2023).

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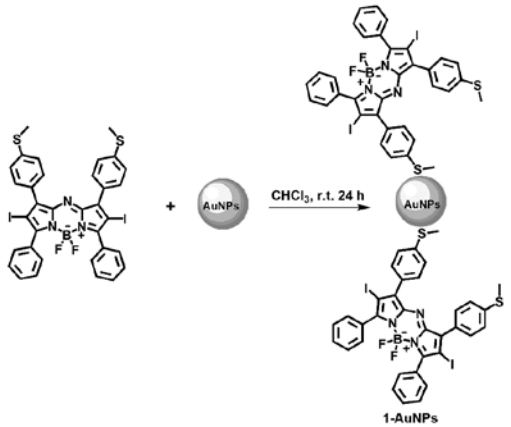


The photodynamic antimicrobial chemotherapy activities of azaBODIPY dyes and their gold nanoparticle conjugates

John Mack, Temlandvo M. Magwaza, Nthabeleng Molupe, Yolande I. Openda, Tebello Nyokong

Tebello Nyokong Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa

Boron dipyrromethene (BODIPY) dyes and their analogues, such as boron dipyrromethene (azaBODIPY), have been studied extensively for dye applications at the red end of the visible and near-infrared [1]. Their photophysicochemical properties can be modified through facile structural modification to enhance their suitability for biomedical photosensitizer dye applications [2]. The synthesis and photophysicochemical properties of two 2,6-diiodinated azaBODIPY dyes with thiomethylphenyl groups at the distal positions and phenyl (**1**) and naphthyl (**2**) rings at the proximal positions are reported. The dyes were conjugated to gold nanoparticles (**1**-AuNPs and **2**-AuNPs) to enhance their aqueous solubility for biomedical applications in a manner similar to what has been reported previously for porphyrin analogues [3, 4].



Iodination at the 2,6-positions of the azaBODIPY core resulted in an enhancement of singlet oxygen generation, with singlet oxygen quantum yield (Φ_Δ) values of 0.82 and 0.55 obtained for **1** and **2**, respectively. The photodynamic antimicrobial chemotherapy (PACT) activities of the dyes were tested with a Thorlabs M660L4 light-emitting diode (LED) against *Staphylococcus aureus* after incubation at 5 μM. Conjugation to gold nanoparticles was found to significantly enhance the PACT activities against *Staphylococcus aureus*. Log_{10} reduction values of 8.94 were obtained for **1**-AuNPs after 30 min irradiation (3.0 $J.cm^{-2}$) and **2**-AuNPs after 60 min (6.0 $J.cm^{-2}$).

REFERENCES

1. Lu H, Mack J, Yang Y, Shen Z. *Chem. Soc. Rev.* 2014; **43**: 4778-4823.
2. Ndundu A, Molupe NR, Sindelo A, Osomba L, K'Ekuboni M, Ngoy BP, Mack J, Nyokong T. *Macroheterocycles* 2024; **17**: 306-314.
3. Soy RC, Babu B, Mack J, Nyokong T, *Dyes Pigments* 2021; **194**: 109631.
4. Magwaza TM, Molupe N, Openda YI, Mack J, Nyokong T. *Photodiagnosis Photodyn. Therapy* 2025; **55**: 104781.

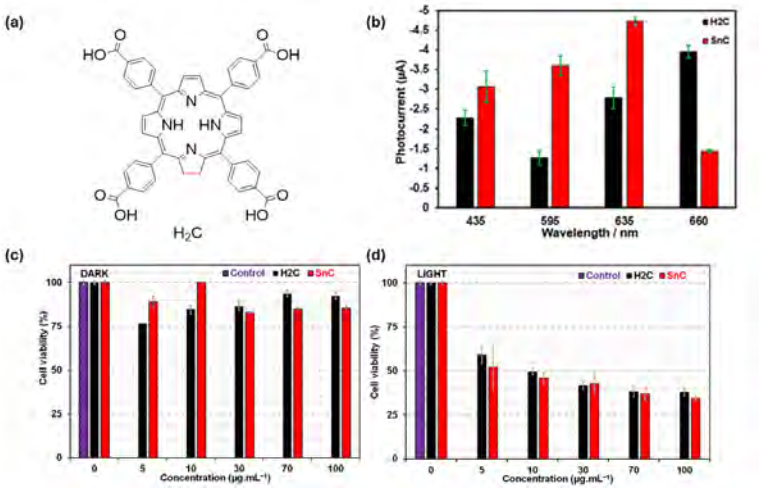
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Novel water-soluble chlorin photosensitizers for use in photoelectrochemistry and photodynamic therapy

John Mack[a], **Mahlatse M. Ledwaba,**[a] **Simone Bassini,**[b,c] **Elise Daems,**[b,c] **Earl Prinsloo,**[d] **Tebello Nyokong,**[a] **Karolien De Wael**[b,c]

[a]*Tebello Nyokong Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa.*
[b]*Antwerp, engineering, photoelectrochemistry, and sensing (A-PECS), Department of Bioscience Engineering, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium.*
[c]*NANOlight Center of Excellence, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium.*
[d]*Biotechnology Innovation Centre, Rhodes University, Makhanda 6140.*

Chlorins have been explored for various applications, such as anticancer and antibacterial photodynamic therapy [1, 2]. However, their application in electroanalysis as photoresponsive materials is still at an early stage [3]. Water-soluble tetra-4-carboxyphenylchlorins have been synthesised and characterised (Figure 1a), including the free base dye (**H_2C**) and its *trans*-axially ligated Sn(IV) complex (**SnC**). **SnC** exhibited high solubility in PBS buffer and a high singlet oxygen ($^1O_2$) quantum yield of 0.70. The chlorins were used in photoelectrochemical studies, with higher photocurrents observed for **SnC** across most of the visible regions (Figure 1b).



Photodynamic therapy activity studies against the MDA-MB-231 breast cancer cell line (Figure 1c-d), a triple-negative, aggressive, and invasive subtype used to model late-stage breast cancer, were conducted through 30 min irradiation with Thorlabs M625L3 (2.6 J.cm^{-2}) and Thorlabs M660L3 (3.0 J.cm^{-2}) LEDs. A favourable IC_{50} value of 5.8 μM was obtained for **SnC**, while a higher value of 12.1 μM was observed for **H_2C**, demonstrating that water-soluble Sn(IV) tetraarylchlorin complexes merit further in-depth study for use as $^1O_2$ photosensitising dyes in biomedical applications.

REFERENCES

1. Babu B, Sindelo A, Mack J, Nyokong T. *Dyes Pigments* 2021; **185**: 108886.
2. Babu B, Mack J, Nyokong T. *Dalton Trans.* 2023; **52**: 5000-5018.
3. Bassini S, Daems E, Sleegers N, De Wael K. *Sensors Actuators B* 2025; **432**: 137387.

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Photophysical Characterisation of Zn(II) and Free-base Pyridiniumporphyrins with a Long Alkyl Chain in Complexes with BSA

Martina Mušković Lukić[a], Martin Lončarić[b], Nikola Basarić[c], Ivana Ratkaj[a], Nela Malatesti[a]

[a]*Faculty of Biotechnology and Drug Development, University of Rijeka, Radmile Matejčić 2, 51000 Rijeka, Croatia*

[b]*Laboratory for Photonics and Quantum Optics, Division of Experimental Physics, Ruđer Bošković Institute, Bijenička Cesta 54, 10000 Zagreb, Croatia*

[c]*Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička Cesta 54, 10000 Zagreb, Croatia*

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Human serum albumin (HSA) is the most abundant protein in blood plasma, and known to form relatively stable complexes with porphyrins. Binding of porphyrin to albumin facilitates their circulation in biological media and promotes passive accumulation in tumours through the enhanced permeability and retention (EPR) effect, improving their localisation and potentially enhancing photodynamic therapy (PDT) outcomes [1].
In our previous work, spectroscopic studies showed that both Zn(II) and free-base porphyrins with long alkyl chains exhibited a broadened, low-intensity Soret band in phosphate buffer, which indicates aggregation. Upon titration with bovine serum albumin (BSA), the Soret band "recovered" its monomeric form, suggesting porphyrin binding to BSA [2]. Although albumin binding is favourable for passive accumulation, it may also alter the photophysical properties of photosensitisers [1], which is still somewhat less studied.
In this work, the aggregation behaviour of Zn(II) and free-base porphyrins with C18 alkyl chains in phosphate buffer and their interactions with BSA was investigated to determine binding constants and the number of porphyrins bound per protein. The singlet and triplet excited-state properties (^{1}PS* and ^{3}PS*) of BSA-bound porphyrins, which are important for photosensitiser activity in biological environments, will be described. In addition, evaluation of singlet oxygen production by monitoring the photodegradation of 1,3-diphenylisobenzofurane (DPBF) and 9,10-anthracenediyl-bis (methylene)dimalonic acid (ABMDMA) will also be presented.

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REFERENCES

1. P. J. Gonçalves, F. C. Bezerra, L. M. Almeida, L. Alonso, G. R. L. Souza, A. Alonso, S. C. Zílio, I. E. Borissevitch, *Eur. BioPhys. J.* **2019**, 48, 721-729.
2. M. Mušković, M. Lončarić, I. Ratkaj, N. Malatesti, *Eur. J. Med. Chem*. **2025**, 282, 117063.

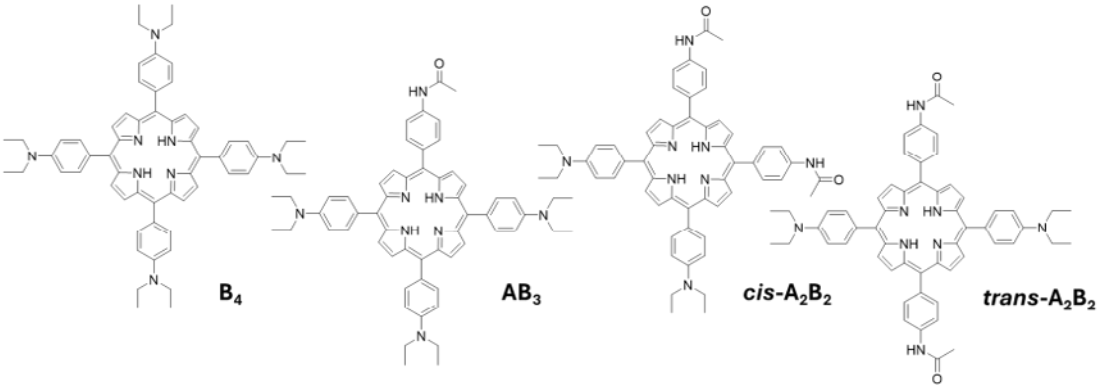
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Photophysics and Hyperporphyrin Effect of New Porphyrins with *N,N*-Diethylaminophenyl and Acetamidophenyl Groups

Martina Mušković[a], Martin Lončarić[b], Nikola Basarić[c], Ivana Ratkaj[a], Nela Malatesti[a]

[a]*Faculty of Biotechnology and Drug Development, University of Rijeka, Radmile Matejčić 2, 51000 Rijeka, Croatia*
[b]*Laboratory for Photonics and Quantum Optics, Division of Experimental Physics, Ruđer Bošković Institute, Bijenička Cesta 54, 10000 Zagreb, Croatia*
[c]*Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička Cesta 54, 10000 Zagreb, Croatia*

The concept of hyperporphyrins was first introduced by Gouterman when he observed a significant bathochromic shift and the appearance of additional bands in the absorption spectra of certain metalloporphyrins, compared to the usual porphyrin spectra [1]. Other examples described so far include hyperporphyrin formation through ligand-to-ligand charge transfer (LLCT) from substituent π to the porphyrin π* system, as a result of the protonation of *meso*-porphyrins with *p*-aminophenyl or *p*-dimethylamino substituents [1,2]. Hyperporphyrins, due to their strong near-infrared (NIR) absorption, could be interesting for photodynamic therapy (PDT) [3], however, to our knowledge, so far, there is not much systematic research showing the potential of that application.
Here we report the synthesis of B_4, and new AB_3 and A_2B_2 porphyrins with *N,N*-diethylaminophenyl and 4-acetamidophenyl substituents as precursors of photosensitizers for PDT, and a study of hyperporphyrin effect by spectroscopic titrations with methanesulfonic acid (MSA) in dimethyl sulfoxide (DMSO) or DMSO/dichloromethane mixture. Their characterization and evidence of hyperporphyrin using ^{1}H NMR spectroscopy will also be presented.



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REFERENCES

1. C. C. Wamser and A. Ghosh, *JACS Au*, **2022**, 2, 1543-1560.
2. C. Wang and C. C. Wamser, *J. Phys. Chem*. **2014**, 118, 3605-3615.
3. J. Conradie, C. C. Wamser and A. Ghosh, *J. Phys. Chem. A*. **2021**, 125, 9953-9961.

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Slurry-State Redox Flow Batteries Employing Silicon Phthalocyanine Oligomers: Electron Delocalization Enhances Cycling Stability

Brendon J. McNicholas[a], **Wren K. J. Stiefel**[b], **Ryan G. Hadt**[b]

[a]*Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37996, United States.*
[b]*Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125, United States.*

The electrochemical characterization and application of silicon phthalocyanine μ-oxo oligomers to symmetric, slurry redox flow batteries are reported. Electrolytes comprising $(C_6H_{13})_3$-Si-O-Si(Pc)-O-Si$(C_6H_{13})_3$, $(C_6H_{13})_3$-Si-O-Si(Pc)-O-Si(Pc)-O-Si$(C_6H_{13})_3$, $(C_6H_{13})_3$Si-O-Si(Pc)-O-Si(Pc)-O-Si(Pc)-O-Si$(C_6H_{13})_3$, Ketjenblack EC-600JD carbon, and $TBAPF_6$ in propylene carbonate exhibit near-unity Coulombic efficiencies and near to greater than 60% energy efficiencies. Notably, $(C_6H_{13})_3$Si-O-Si(Pc)-O-Si(Pc)-O-Si(Pc)-O-Si$(C_6H_{13})_3$ exhibits negligible capacity fade over two weeks of charge-discharge cycling at 50% state of charge. The unique multi-electron oxidative stability of higher-order oligomers is rationalized through a combination of time-dependent density functional theory (TDDFT) and *ab initio* calculations. These materials provide a promising class of multi-electron transfer reagents for use in semi-solid, non-aqueous redox flow batteries.

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Electronic Characteristics of Cyano-Substituted Transition Metal Tetraphenylporphyrins

Brendon J. McNicholas[a], **Emma E. Lane**[a], **and Marissa N. Kuruce**[a]

[a]*Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37996, United States.*

Transition metal porphyrins, particularly those of the first row, have been at the forefront of various electrocatalytic and photocatalytic processes due to their structural resemblance to naturally occurring porphyrinoid active sites. It is imperative to understand the electronic structures of these species to optimize performance in such catalytic reactions. We performed a comprehensive spectroscopic, electrochemical, and theoretical examination of several first row transition metal tetraphenylporphyrins (M = Fe, Mn, Cr, Cu), specifically those with *para*-cyano substituents. UV-vis-NIR spectroscopy and magnetic circular dichroism in combination with TDDFT calculations were used to identify energies of various charge transfer bands of the ground state species. Spectroelectrochemical experiments evaluated the character of reduction and oxidation events of these porphyrins, evinced by cyclic voltammetric studies. Determination of such events as either porphyrin or metal centered is valuable in understanding behavior for these complexes in electrocatalytic applications. Comparison to previously reported spectra and assignments of other transition metal tetraphenylporphyrins demonstrates that cyano-substitution alters the identities of certain redox events in both coordinating and non-coordinating solvents (DMF and DCM). Additionally, we make assignments for previously underreported second, third, and fourth reduction and oxidation events for certain metalloporphyrins in this study in both solvents. These assignments will further understanding of the electronic characteristics of substituted transition metal porphyrins for use in electro- and photocatalytic processes.

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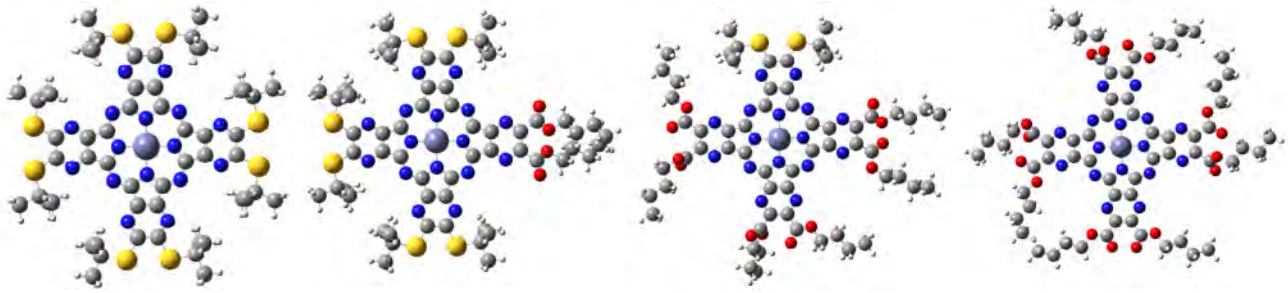


Characterization of the effects of peripheral substitutions on the electronic structure of tetrapyrazinoporphyrazines

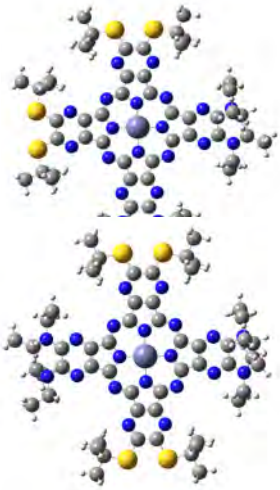
Dennis Mercier[a], **Veronika Nováková**[b], **and Martin J. Stillman**[a]

[a]*The University of Western Ontario, Department of Chemistry, London, ON N6A 3K7, Canada*
[b]*Charles University, Faculty of Pharmacy, Ak. Heyrovskeho 1203, 500 03 Hradec Kralova, Czech Republic*

Computational chemistry has been employed to investigate the theoretical and optical characteristics of a range of zinc tetrapyrazinoporphyrazines (ZnTPyPzs) [1], as a function of a series of spatially distributed, electronically active substituents (-$SC(CH_3)_3$; -$COOC_4H_9$) on the electron-rich ring:



Molecular Orbital (MO) analysis, depicting the surface distribution of electronic charge, has revealed intriguing patterns in nominally forbidden transitions that influence the optical properties. UV-visible absorption spectra and magnetic circular dichroism (MCD) measurements have been complemented by theoretical calculations to elucidate the complex changes in both the B- and Q-band regions. Theoretical analysis overcomes the muddying effects of the overlapping charge transfer (CT) bands in the assignment of π to π* transitions, leading to the characterization of the individual MOs involved in each of the excited states.



We also report the effect on the electronic structure of the substitution in an AABB pattern (right top) compared to an ABAB pattern (right bottom) for the ZnTPyPzs.

The observed spectroscopic data for ABAB is accounted for by an unusual split of the energies of the LUMO and LUMO+1 in contrast to the near degeneracy of the LUMO and LUMO+1 in AABB. These results complement the conclusions previously reached for substituted phthalocyanines using ZINDO/S methods [2].

REFERENCES

1. Novakova, V., J. Porphyrins Phthalocyanines, **26**, 765-782 (2022)
2. Kobayashi, N., Mack, J., Ishii, K., Stillman. M.J., Inorg. Chem., **41**, 5350-5363 (2002)

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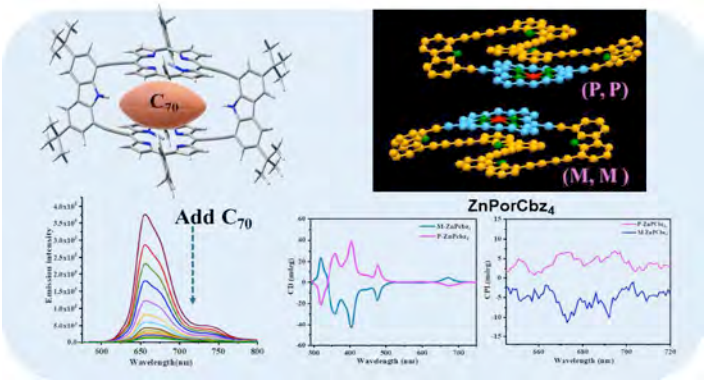
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Porphyrin-Carbazole Architectures: From Selective Fullerene Recognition to Topologically Interesting Chiral Macrocycles

Mohini Mittal,[a] Sameeksha Agarwal,[a] Pradeep Kumar Mondal,[b] Jeyaraman Sankar*[a]

[a] *Department of Chemistry, Indian Institute of Science Education and Research Bhopal (IISER Bhopal), Bhopal Bypass Road, Bhopal 462066, India.*
[b] *Elettra-Sincrotrone Trieste, Strada Statale 14 km 163.5 in Area Science Park, 34149 Basovizza, Trieste, Italy.*

Shape-persistent, three-dimensional π-conjugated molecular architectures have emerged as versatile platforms for applications in host-guest chemistry, molecular electronics, and chiral photonic materials. [1a,1b] Fullerene has sparked intense research interest due to its unique electron-accepting properties and applications in photovoltaics, electronics, and biopharmaceutical industries.[1c] However, the difficulties in purifying, solubilizing, and derivatizing fullerenes can be overcome through p-electronic donor-acceptor interactions during complexation in host-guest chemistry. Noncovalent complexation with electron-rich π-donor hosts offers an effective strategy to address these limitations while maintaining the intrinsic electronic properties of fullerenes.[2a] Porphyrins are well-suited in this context due to their large π-surface area, strong donor properties, intense visible-to-near-infrared optical transitions, and exceptional chemical and thermal stability. In parallel, recent advances in fully π-conjugated macrocycles have highlighted the emergence of chirality from rigid molecular topologies, such as figure-eight architectures, in which chirality arises from global connectivity rather than from classical stereogenic elements.[2b] The development of rigid porphyrin-based π-conjugated frameworks will be discussed, highlighting selective fullerene recognition[3a] and enhanced chiroptical responses[3b] with potential applications in molecular electronics and optoelectronics.



REFERENCES

1. (a) Rebek, J., Jr. Agnew. Chem., Int. Ed. **2005**,*44*,068–2078; (b) Inokuma, Y.; Kawano, M.; Fujita, M. Nat. Chem. **2011**,*3*,349–358: (c) Pivrikas, A.; Sariciftci, S. N.; Juska, G.; Osterbacka, R. Prog. Photovoltaics **2007**,*15*,677.
2. (a) Tashiro, K.; Aida, T.; Zheng, Y. J.; Kinbara, K.; Saigo, K.; Sakamoto, S.; Yamaguchi, K. J. Am. Chem. Soc. **1999**,*121*,9477–9478; (b) Kubo, H.; Shimizu, D.; Hirose, T.; Matsuda, K. *Org. Lett.* **2020**, *22*, 9276-9281.
3. (a) **Mittal, M.;** Agarwal, S.; Mondal, P. K.; Polentarutti, M.; Sankar, J. ChemRxiv [Preprint] 2025. (b) **Mittal, M. ;** Mondal, P. K. ; Sankar, J. *Manuscript under preparation.*

POSTERS

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Charge Transport Properties of a Tetrabenzoporphyrin Derivative with the Superlattice Herringbone Structure

Kazuya Miyazaki[a], Keitaro Yamamoto [a], Mitsuaki Yamauchi [a], Yoshiyuki Mizuhata [a], Hiroko Yamada [a]

[a]*Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*

In organic field-effect transistors (OFETs), precise control of crystal packing is essential for realizing two-dimensional charge-transport pathways and achieving high charge-carrier mobility. Among various packing motifs, the herringbone (HB) structure is known to afford efficient lateral transport. We have previously demonstrated that substituent-controlled HB packing in tetrabenzoporphyrins (TBPs) leads to high hole mobilities in OFETs [1-3].

In this study, we report the charge-transport properties of a unique superlattice HB structure formed via a solvent-desorption-induced single-crystal-to-single-crystal (SCSC) transformation. 5,15-Bisphenyl-tetrabenzoporphyrin (**Ph-TBP**) forms a cocrystal composed of alternating layers of HB-packed **Ph-TBP** and *o*-dichlorobenzene (*o*-DCB) upon low-temperature recrystallization from an *o*-DCB/THF solution. Subsequent vacuum heating removes the intercalated *o*-DCB molecules and induces a structural transformation in which alternating **Ph-TBP** layers rotate by 90°, resulting in a superlattice composed of two orthogonally oriented HB packings.

Marcus hopping calculations predict favorable two-dimensional charge transport within both constituent layers of the superlattice. Single-crystal bottom-gate top-contact OFETs fabricated on Si/SiO_2 substrates exhibit anisotropic hole mobilities of 3.8 ± 1.8 $cm^2\ V^{-1}\ s^{-1}$ and 1.5 ± 0.5 $cm^2\ V^{-1}\ s^{-1}$ along the b- and c-axes, respectively. Notably, the maximum mobility reaches 11.3 $cm^2\ V^{-1}\ s^{-1}$, which is the highest value reported for porphyrin-based semiconductors. Detailed crystal structures, device fabrication procedures, and charge-transport characteristics will be presented.

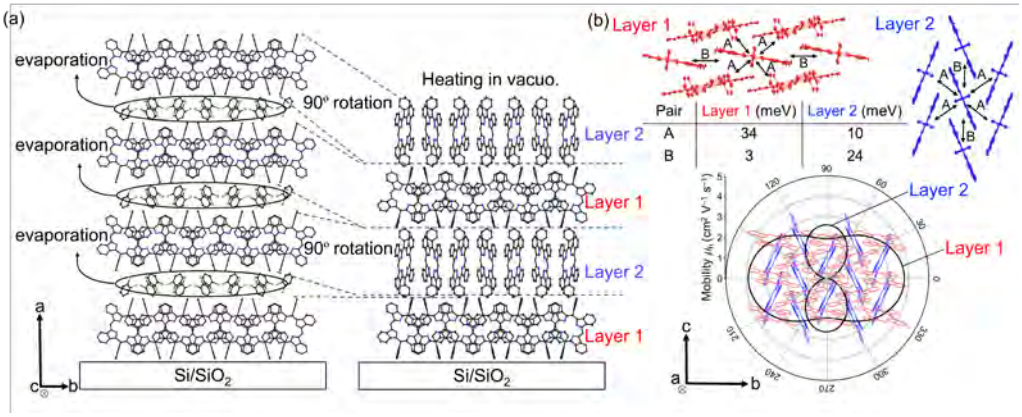


Figure 1. (a) SCSC transformation from the cocrystal of **Ph-TBP** with *o*-DCB to superlattice HB structure formed on a substrate. (b) Calculated charge-transfer integrals and theoretical charge-carrier mobilities based on the Marcus hopping model for each layer.

REFERENCES

1. K. Miyazaki et al. *Org. Lett.* **2023**, 25, 7354.
2. K. Miyazaki et al. *Adv. Mater. Interfaces* **2025**, 12, 2400946.
3. K. Miyazaki et al. *J. Porphyr. Phthalocyanines* **2025**, 29, 213.

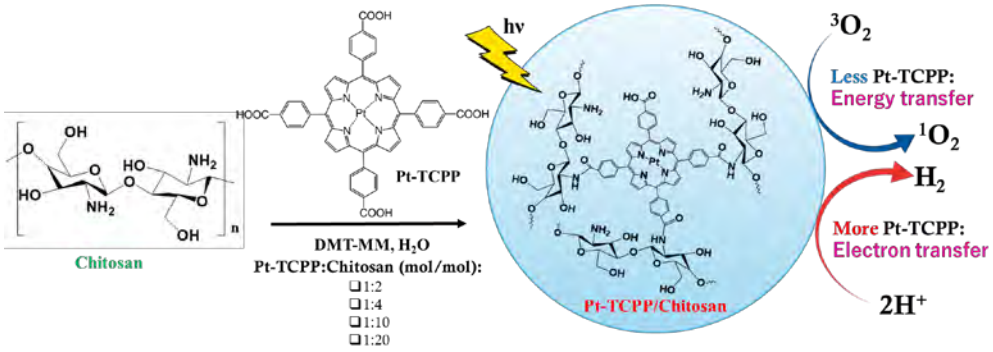
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Tuning Photo-excited Pathways of Platinum (II)-Porphyrin by Chitosan for an Efficient Photocatalyst

Kushal Mohan Gowda[a], Yasuko Osakada[b, c], Mamoru Fujitsuka[b, c], Vasudevanpillai Biju[a, d], Yuta Takano[a, d]

[a] *Graduate School of Environmental Science, Hokkaido University, Sapporo, Japan*
[b] *SANKEN (The Institute of Scientific and Industrial Research), The University of Osaka, Ibaraki, Japan*
[c] *Open and Transdisciplinary Research Initiatives (ICS-OTRI), The University of Osaka, Suita, Japan*
[d] *Research Institute for Electronic Science, Hokkaido University, Sapporo, Japan*

The reactivity of molecular photocatalysts in nature is governed by sophisticated microenvironments, yet mimicking these in an artificial system remains challenging. Metalloporphyrins, with their unique photophysical and photoredox properties, are widely employed in artificial photocatalytic systems for solar energy conversion. Nevertheless, Pt(II) meso-tetrakis(4-carboxyphenyl) porphyrin (Pt-TCPP), despite having a Pt metal centre, remains largely unexplored in synthetic photocatalysis because of its tendency to aggregate in aqueous media, which often limits its efficiency. The incorporation of porphyrins into biopolymer matrices, such as chitosan, offers a way to stabilize the chromophores and improve its dispersibility. Chitosan, a natural biopolymer containing abundant amine and hydroxyl functional groups, can serve as a sustainable support capable of suppressing the aggregation of photosensitizers [2]. Notably, the use of chitosan has been reported to enhance photocatalytic hydrogen evolution [3], emphasizing its ability to improve both stability and activity.



Scheme. Syntheses of Pt-TCPP/chitosan conjugates with switchable photoactivity.

Herein, we prepared a hybrid photocatalytic system by grafting varying equivalents of Pt-TCPP (0.50, 0.25, 0.10, and 0.050 eq.) on chitosan scaffolds (Pt-TCPP/chitosan), enabling cocatalyst-free functioning (**Scheme**).

Under blue light irradiation with ascorbic acid in an aqueous medium, 0.50 eq. conjugate exhibited remarkable photo-reductive activity, achieving an H_2 generation rate of 88 mmol g^{-1} h^{-1}, the highest level for such systems. Interestingly, by reducing the Pt-TCPP density on chitosan ($\leq$ 0.10 eq.) the system shifts towards the energy transfer pathway, efficiently producing singlet oxygen ($^1O_2$). Overall, the PtTCPP/chitosan hybrid system allows the controlled modulation of photoexcited pathways, offering a co-catalyst-free sustainable platform for solar energy harvesting.

REFERENCES

1. J.-X. Jian *et al.*, *Nat. Commun.*, 2013, *4*, 2695.
2. A. Charisiadis *et al.*, *Chem. Commun.*, 2025, *61*, 4630.
3. C. P. Jiménez-Gómez and J. A. Cecilia, *Molecules,* 2020, *25*, 3981.

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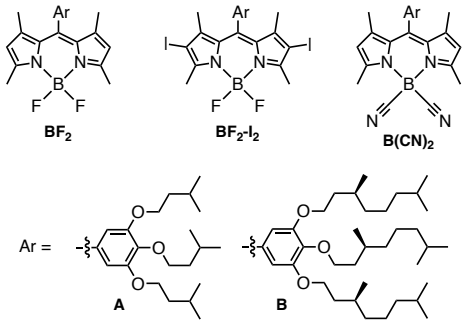
Interface-Induced Modulation of Fluorescence in Liquid and Semicrystalline BODIPYs

Mitsuhiko Morisue[a], Masashi Yamaguchi[a], Takahito Shibahara[a], Hiroaki Harada[b], Ken-ichi Yuyama[c], Masashi Nakamura[d], Yukiyasu Kashiwagi[d], Hiroyasu Masunaga[e], Sono Sasaki[f,g], Munetaka Iwamura[b], Koichi Nozaki[b], and Tatsuo Taniguchi[h]

[a]*Faculty of Molecular Chemistry and Engineering, Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan*
[b]*Graduate School of Science and Engineering, University of Toyama, 3190 Gofuku, Toyama 930-8555, Japan*
[c]*Department of Chemistry, Graduate School of Science, Osaka Metropolitan University, 3-3-138 Sugimoto, Osaka 558-8585, Japan*
[d]*Osaka Research Institute of Industrial Science and Technology, 1-6-50 Morinomiya, Joto-ku, Osaka 536-8553, Japan*
[e]*Japan Synchrotron Radiation Research Institute (JASRI/SPring-8), Hyogo 679-5198, Japan*
[f]*Faculty of Fiber Science and Engineering, Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan*
[g]*RIKEN SPring-8 Center, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5148, Japan*
[h]*Depaerment of Applied Chemistry and Biotechnology, Graduate School of Engineering, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan*

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The considerable conformational entropy of branched alkyl chains, such as 3,4,5-tris(isopentyloxy)phenyl and 3,4,5-tris((*S*)-dihydrocitronellyloxy)phenyl groups, actively modulates the morphological properties of BODIPYs, offering a new materials perspective for BODIPY assemblies. Poor mutual immiscibility between the rigid BODIPY core and the branched alkyl chains drives segregation into lamellar structures. Notably, iodinated BODIPY **BF_2-I_2-A** and **BF_2-I_2-B** formed J-aggregate in spin-coated films characterized by remarkably sharp absorption, and single crystal analysis of **BF_2-I_2-A** elucidated the underlying molecular packing. In contrast, BODIPY **BF_2-B** showed persistent fluidity at ambient temperature under solvent-free conditions. Interestingly, the fluorescence properties of a bar-coated film of **BF_2-B** on a quartz substrate drastically changed when it was sandwiched between quartz slides. Similar alternations in fluorescence properties were observed for **$B(CN)_2$-B**, which undergoes cold crystallization at 29.5 °C below its melting point at 70.0 °C. This anomalous fluorescence behavior may arise from interfacial effects. The Gibbs–Thomson effect, a representative thermal effect arising from Laplace pressure, lowers the melting point relative to the bulk when the crystal size is smaller than 1 μm. To investigate this effect, nanoporous siloxane films were fabricated using monodisperse polymer nanoparticles as templates. As diameter of nanopores decreased below 2 μm, the J-aggregate content of **$B(CN)_2$-B** gradually diminished and an amorphous state emerged. Furthermore, thermal treatment of a bar-coated film of **$B(CN)_2$-B** induced dewetting from quartz surface. Gradual cooling crystallized the molten droplets into spherulites with a characteristic Maltese cross. Consequently, the microdroplets involved a hierarchical crystal-in-glass structure. An increase in droplet diameter from 10 to 40 μm enhanced the ratiometric fluorescence intensity of the J-aggregate at 568 nm compared with the dimeric species at 745 nm.



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A_2B_2-type porphyrins bearing nitrogen-donor units: Synthesis and photo-antibacterial efficiency

Melani J. A. Reis[a], Cátia Vieira[b], M. Graça P. M. S. Neves[a], Adelaide Almeida[b], M. Amparo F. Faustino[a], Nuno M. M. Moura[a]

[a] *LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal*
[b] *CESAM, Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal*

The rapid emergence of antimicrobial resistance has intensified interest in antimicrobial photodynamic therapy (aPDT) as an alternative to conventional antibiotics. aPDT relies on the activation of a photosensitiser (PS) by visible light in the presence of dioxygen, leading predominantly to the generation of singlet oxygen ($^1O_2$) and other reactive oxygen species (ROS) capable of inducing multi-site oxidative damage in microbial cells.[1] Owing to this multitarget mode of action, aPDT enables the efficient inactivation of a broad spectrum of pathogenic microorganisms, including highly drug-resistant strains.[2,3]
The efficacy of aPDT is critically dependent on the photophysical and photochemical properties of the PS, positioning porphyrins as leading molecular platforms due to their strong absorption, high $^1O_2$ generation efficiency, and structural tunability.
In this communication, as alternative PSs to the commonly used *meso*-tetrarylporphyrin, we will discuss the synthesis of a series of free-base and Zn(II) complexes of *trans*-A_2B_2-type porphyrins, bearing different nitrogen-based donor groups (carbazole, 3,6-dimethoxy-9*H*-carbazole, 10*H*-phenoxazine, 10*H*-phenothiazine and bis(4-methoxyphenyl)amine) directly linked to the macrocycle via C–N bonds.Their further incorporation into polyvinylpyrrolidone (PVP) formulations and the assessment of their antimicrobial photodynamic activity against the Gram-positive bacterium *Staphylococcus aureus* will also be discussed.[4]

Funding/Acknowledgements: This research work received financial support from the University of Aveiro and FCT/MCTES to support UID/50006/2023 - Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos and CESAM (LA/P/0094/2020) research units, and to the Portuguese NMR Network. MJA Reis acknowledges FCT for her doctoral grant (2020.05838.BD) and NMM Moura for an Assistant Research Position under the Individual Scientific Employment Stimulus - 6th Edition (2023.06495.CEECIND).

REFERENCES

1. Piksa, M., Lian, C., Samule, I.C., Pawlik, K.J., Samuel, I.D.W., Matczyszyn, K. The role of the light source in antimicrobial photodynamic therapy. *Chem. Soc. Rev.* **2023**, *52*, 1697-1722.
2. Vieira C., Gomes, A.T.P.C., Mesquita, M., Moura, N.M.M., Neves, M.G.P.M.S., Faustino, M.A.F., Almeida, A. An insight into the potentiation effect of potassium iodide on aPDT efficacy. *Front. Microbiol.* **2018**, *9*, 2665.
3 Mesquita, M., Dias, C.J., Neves, M.G.P.M.S., Almeida, A., Faustino, M.A.F. Revisiting current photoactive materials for antimicrobial photodynamic therapy, *Molecules.* **2018**, *23*,2424.
4. Reis, M.J.A., Vieira, C., Bartolomeu, M., Faustino, M.A.F., Pereira, A.M.V.M., Neves, M.G.P.M.S., Almeida, A., Moura, N.M.M. A_2B_2-type porphyrins enhanced by N-donor units: synthesis optimization and photodynamic efficiency towards *S. aureus*. *Bioorg. Chem.* **2025**, *162*, 108607.

POSTERS

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Development of porphyrin-silica adsorbents for efficient toxic metal ions removal from industrial wastwater

Chahrazad El Abiad[b], Smaail Radi[b], M. Amparo F. Faustino[a], M. Graça P. M. S. Neves[b], Nuno M. M. Moura[a]

[a] *LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal*
[b] *Mohammed First University, Faculty of Sciences, LCAE, 60 000 Oujda, Morocco.*

Current wastewater treatment facilities face a growing challenge due to the presence of emerging contaminants, such as industrial chemicals, hormones, and personal care products, alongside hazardous heavy metals. This has created a critical global demand for technologies capable of efficiently removing these pollutants.[1] In particular, long-term exposure to toxic metal ions, such as Cu^{2+}, Pb^{2+}, Cd^{2+}, and Zn^{2+}, poses significant threats to human health, including organ damage, interference with hemoglobin production, cancer and impaired cognitive development. While several techniques exist to purify contaminated water, such as chemical precipitation, ion exchange, and osmosis, adsorption is widely considered the most advantageous method. It is favored for its high efficiency, ease of operation, low cost, and environmentally friendly nature.[2]
From the available adsorption supports, mesoporous silica gel has attracted considerable attention due to its high surface area, large pore volume, thermal stability, and low toxicity.[3] Its performance can be further enhanced by functionalization with chelating ligands such as porphyrins, well known by their strong metal-binding ability and improved selectivity toward target metal ions.[4]
This communication reports the development and characterization of silica-based inorganic-organic hybrid materials featuring different *meso*-tetraarylporphyrin ligands and discusses how their structural features influence their performance as adsorbents for industrial water purification and the removal of toxic metals.

Funding/Acknowledgements: This research work received financial support from the University of Aveiro and FCT/MCTES to support UID/50006/2023 - Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos and CESAM (LA/P/0094/2020) research units, and to the Portuguese NMR Network. NMM Moura thanks FCT for an Assistant Research Position under the Individual Scientific Employment Stimulus - 6th Edition (2023.06495.CEECIND). The authors extend their appreciation to the PPR2-MESRSFC-CNRST-P10 project (Morocco) for the financial support.

REFERENCES

1. Rizzo, L., Addressing main challenges in the tertiary treatment of urban wastewater: are homogeneous photodriven AOPs the answer? *Environ. Sci. Water Res. Technol.* **2022**, *8* , 2145.
2. Kumar, R., Laskar, M.A., Hewaidy, I.F., Barakat, M.A. Modified Adsorbents for Removal of Heavy Metals from Aqueous Environment: A Review. *Earth Syst. Environ.* **2019**, *3*, 83-93.
3. Radi, S., Chahrazad, E.A., Moura, N.M.M., Faustino, M.A.F.,M., Neves, M.G.P.M.S. An efficient hybrid adsorbent based on silica-supported amino penta-carboxylic acid for water purification. *J. Mater. Chem. A* **2018**, *6*, 13096-13109.
4 Chahrazad, E.A., Radi, S., El Massaoudi, M., Lamsayah, M. Figueira, F., Faustino, M.A.F.,M., Neves, M.G.P.M.S., Moura, N.M.M. Porphyrin-silica gel hybrids as effective and selective copper(II) adsorbents from industrial wastewater. *J. Env. Chem. Eng.* **2023**, *11*, 110097.

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Cobalt (II) and Cobalt (III) Phthalocyanine Amine Complexes

Breanna E. Muldowney[a], Benjamin C. Childs[a], Michael D. Gutiérrez[a], Michael P. Hendrich[b], Viktor N. Nemykin[a]

[a]*Department of Chemistry, University of Tennessee – Knoxville, Knoxville, TN USA (bmuldow1@vols.utk.edu)*
[b]*Department of Chemistry, Carnegie Mellon University, Pittsburgh, PA USA*

Transition metal phthalocyanines are generally known in literature for applications in photo- and electrocatalysis; thus necessitating in-depth studies into effects of L-/X- type axial ligands on the phthalocyanine metal center. A large series of cobalt (II) and cobalt (III) phthalocyanine complexes with axial coordination of alkyl- and aryl-amines have been investigated by a variety of experimental (UV-vis-NIR, Magnetic Circular Dichroism, Electronic Paramagnetic Resonance, Spectroelectrochemistry, Nuclear Magnetic Resonance, and X-Ray Diffraction) and theoretical (DFT, TDDFT) methods [1]. By using amines of varying basicity and steric properties such as n-butylamine, isobutylamine, isopropylamine, *sec*-butylamine, *tert*-butylamine, pyridine, piperidine, 4-dimethylaminopyridine, and morpholine allows us to discuss general spectroscopic trends and redox properties of multiple $PcCo^{II}(L)_2$ and $PcCo^{III}(L)_2$ species.

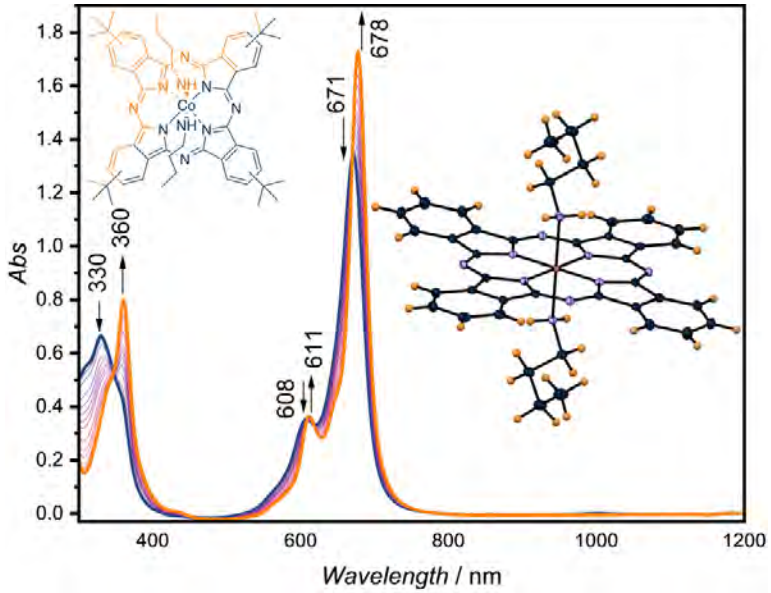


Figure 1. Spectroelectrochemical UV-vis-NIR oxidation of $Pc^{tBu}(2\text{-})Co^{II}(nBuNH_2)_2$ to $[Pc^{tBu}(2\text{-})Co^{III}(nBuNH_2)_2]^+$ in 0.3 M [TBA](ClO_4)/DCM; also shown crystal structure of the $[Pc^{tBu}(2\text{-})Co^{III})(nBuNH_2)_2]^+$ species obtained via XRD.

REFERENCES

1. Muldowney, B. E.; Nevonen, D. E.; Jeaydi, T. I.; Ziegler, C. J.; McNicholas, B. J.; Nemykin, V. N. Identifying charge transfer and trip-multiplet states in Co(I), Co(II), and Co(III) phthalocyanines using (magneto)optical spectroscopy and (TD)DFT calculations. *Dalton Trans.* **2025**, 54, 8846-8869.

POSTERS

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Coordination-Induced Porphyrin Dimers with an Expanded Cavity as Host Molecules

Yuto Nakaie[a], Ryota Yamada[a] Joe Otsuki[a]

[a] *College of Science and Technology, Nihon University, Japan*

Face-to-face porphyrin dimers have been actively studied for applications as host molecules and catalysts. In our laboratory, Recently, we reported a face-to-face porphyrin dimer formed by adding zinc ions to porphyrins with bipyridine or phenanthroline groups (Figure 1) [1, 2]. However, the distances between the two porphyrin planes in this these dimers are too short to accommodate any guest molecules. In this study, we designed a new porphyrin structure with two acetylene units as spacers. This design increases the distance between the porphyrin planes in the dimer, allowing guest molecules to be encapsulated and giving the dimer a host function. Dimer formation was confirmed by UV-vis spectroscopy and ESI-MS data in the presence of Zn^{2+}. UV-vis titration indicates strong binding of 4,4'-bipyridine in this porphyrin dimer with an expanded internal cavity. The binding constant was on the order of 10^5 M^{-1}, which is roughly two-orders of mangitude larger than that for 4,4'-bipyridine binding to the monomer or for 4-phenylpyridine binding to the dimer. This strong binding indicates that 4,4'-bipyridine is encapsulated in the dimer through two-point Zn-N coordination inside the porphyrin cavity.

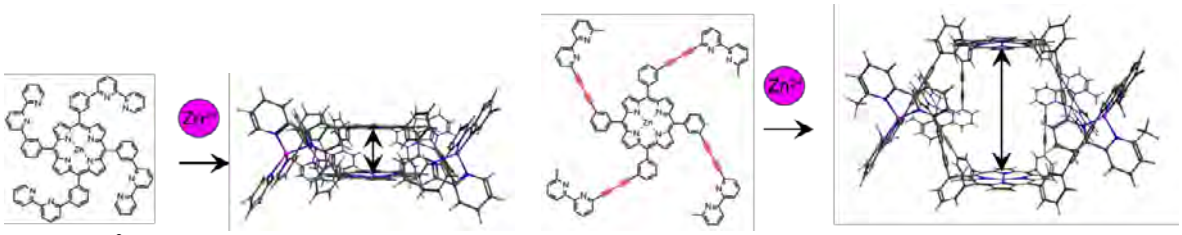


Figure 1. Zn^{2+}-induced face-to-face dimer formation of porphyrins bering bipyridine side chains.

REFERENCES

1. J. Otsuki *et al., Eur. J. Inorg. Chem*., **2024**, *27*, e202400188.
2. J. Otsuki *et al*., *Chem. Lett.*, **2025**, *54*, upaf182.

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Synthesis and Photophysical Properties of *β,β*-Butadiyne-bridged BODIPY Nanorings

Tomokazu Nakamura[a], Masatoshi Ishida[a]

[a]*Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University, Hachioji 192-0397 Japan*

π-Conjugated nanohoop molecules have attracted considerable attention because of their unique photophysical and electronic properties arising from their curved π-electron frameworks, size-dependent optical characteristics, and host–guest interactions.[1] In particular, advances in the synthesis of rigid macrocyclic molecules such as cycloparaphenylenes and cycloparaphenylene acetylenes have enabled the development of valuable functional materials, including circularly polarized luminescent dyes, bioimaging probes, and templates for carbon materials.[2]

From the standpoint of molecular engineering and the functional design of π-conjugated systems, the incorporation of functional π-electronic units into nanohoop skeletons represents a rational strategy for constructing structurally well-defined architectures with tunable optical properties. Inspired by the half-skeleton structure of porphyrin nanorings reported by Anderson and co-workers,[3] we designed a tetrameric BODIPY nanohoop **B₄** composed of β,β-butadiyne-bridged units in this work (Figure 1). The resulting BODIPY nanoring is expected to exhibit strong light-harvesting ability and a large molar absorption coefficient, owing to effective polarization along its cyclic π-conjugated framework. Moreover, its photoresponse wavelength can be tuned from the visible to the near-infrared region through substituent modification.

In fact, the cyclic BODIPY tetramer, **B₄** shows the relatively small strain energy of approximately 20.8 kcal mol^{-1} based on homodesmotic reaction analysis at the DFT (B3LYP) level of theory. Furthermore, optical measurements of **B₄** in CH_2Cl_2 revealed a tailing absorption feature and remarkably broad fluorescence with a large Stokes shift (2754 cm^{-1}) (Figure 1). The detailed synthesis of nanoring **B₄** and the photophysical properties arising from its cyclic structure will be discussed in this presentation.

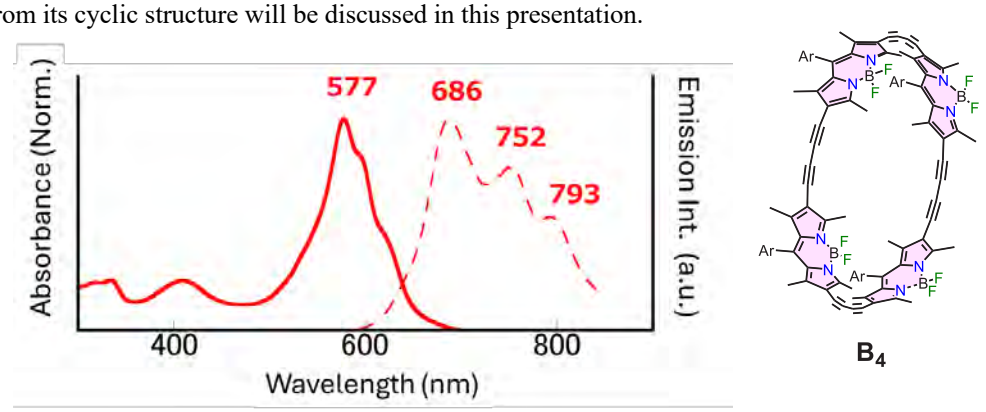


Figure 1. Absorption (solid line) and Emission (broken line) spectra of **B₄** in CH_2Cl_2

REFERENCES

[1] B. Esser *et al*., *Angew. Chem. Int. Ed*. **2021**, *60*, 15743.
[2] R. Jasti *et al*., *Nat. Rev. Chem*. **2019**, *3*, 672.
[3] H. L. Anderson *et al*., *Angew. Chem. Int. Ed*. **2008**, *47*, 4993.

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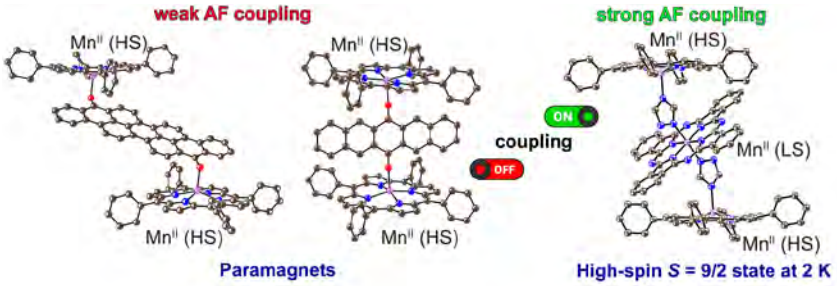
Binuclear Coordination Assemblies of Metal Tetraphenylporphyrins (M = Mn, Fe, and In) with various Dyes (thioindigo, pentacenequinone, *iso*-violanthrone, and manganese(II) phthalocyanine)

Nazarov D.I.[a], Faraonov M.A. [a], Konarev D.V. [a]

[a]*Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Moscow region,142432 Russia*

Metalloporphyrins are widely used in medicine, materials science, biomimetic chemistry, catalysis, and organic photovoltaics. We developed synthetic approaches to coordination compounds of metal tetraphenylporphyrins (M = Mn, Fe, In) with organic dyes in different redox states, including *iso*-violanthrone, pentacenequinone, MnII(triazole)$_2$Pc, and thioindigo radical anions and dianions. The key role of bridging ligands in mediating magnetic exchange in 2Mn^{II}TPP•L systems was demonstrated. The properties of these complexes can be effectively tuned by varying the bridging ligands. In the 2MnTPP–Mn^{II}(triazole)$_2$Pc complex, strong antiferromagnetic coupling between high-spin Mn^{II}TPP centers and the low-spin Mn^{II}Pc unit is observed ($J = -35.2$ cm^{-1}), leading to a high-spin ground state $S = 9/2$ at 2 K. Among the most intriguing findings, two MnTPP complexes with thioindigo radical anions were obtained, differing in porphyrin–thioindigo dihedral angles (90° and 35°). In both systems, Mn^{2+} and Mn^{3+} centers interact differently with the radical anion bridge, as reflected in the exchange parameters ($J_1 = +9.5$, $J_2 = +7.9$, $J_3 = +3.7$ cm^{-1} for 90°; $J_1 = +1.6$, $J_2 = -0.8$, $J_3 = -0.3$ cm^{-1} for 35°). The orthogonal geometry exhibits dominant ferromagnetic exchange, whereas deviation from orthogonality weakens interactions and results in antiferromagnetic coupling of spins.

The suggested method of preparation of multi-chromophore self-assembly hybrids opens significant prospects in material design since different dyes and macrocycles can be combined. A wide variety of these components can lead to complexes with diverse optical, magnetic and even conductive properties..



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REFERENCES

1. Nazarov D.I., Faraonov M.A., Konarev D.V., et al., Dyes and Pigments **2024**, 223, 111926.
2. Nazarov D.I., Faraonov M.A., Konarev D.V., et al., Inorganic Chemistry **2024**, 63, 22677-22687.

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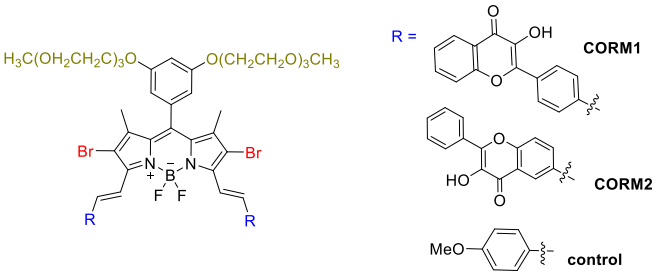


NIR Absorbing BODIPY-Flavonol Conjugates as CO Releasing Molecules

Nidhi Nehra,[a] Veronika Novakova,[a] Petr Zimcik[a]

[a] *Department of Pharmaceutical Chemistry and Pharmaceutical Analysis, Faculty of Pharmacy in Hradec Králové, Charles University, Akademika Heyrovskeho 1203, Hradec Králové 50003*

Carbon monoxide (CO) is an endogenous signalling molecule which plays a crucial role in various biological processes, including cellular signalling, ischemia reperfusion injury, anti-inflammatory, anti-coagulation etc [1]. Among the photoactivable CO releasing molecules (photoCORMs), most common are transition metal based photo CORMs but their acute metal toxicity and poor solubility limit therapeutic applications. To overcome these drawbacks, photoactivable metal free organic molecules-based CORMs have been explored in literature [2-3]. In this regard, we have designed and synthesized the BODIPY photoCORMs (CORM1, CORM2) functionalized with 3-hydroxy flavonol units at 3,5- positions of the bodipy core via knoevenagel condensation reaction for the extended conjugation. PEG units are incorporated at the meso position of BODIPY core to facilitate water solubility and biocompatibility, while bromine atoms are introduced for the enhanced ISC and singlet oxygen production. Moreover, BODIPY dyes are known for their sharp absorption, high fluorescence quantum yield, and excellent photostability, making them ideal scaffolds for designing photoresponsive systems. The synthesized compounds were thoroughly characterized by ^{1}H, ^{13}C NMR spectroscopy, and mass spectrometry. The preliminary photophysical properties were investigated by UV-Vis absorption, fluorescence emission, lifetime, quantum yield measurement, along with singlet oxygen studies. The obtained results proved that CO release occurs, but substatnital differences between the derivatives were observed.



Scheme 1: Representation of the synthesized Bodipy-Flavonol conjugates.

This work was supported by the project New Technologies for Translational Research in Pharmaceutical Sciences /NETPHARM, project ID CZ.02.01.01/00/22_008/0004607, co-funded by the European Union

REFERENCES

1. Marhenke, J.; Trevino, K.; Works, C. *Coord. Chem. Reviews* **2016**, *306*, 533-543.
2. Palao, E.; Slanina, T..; Muchova, L.; Solomek, T.; Vitek, L.; Klan, P. *J. Am. Chem. Soc.* **2016**, 138, 1, 126–133.
3. Ramundo, A.; Janos, J..; Muchova, L.; Srankova, M.; Slavicek, P.; Klan, P. *J. Am. Chem. Soc.* **2024**, 146, 920-929.

POSTERS

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Overcoming thermodynamic limitations in red-light reactions utilizing interatomic interactions

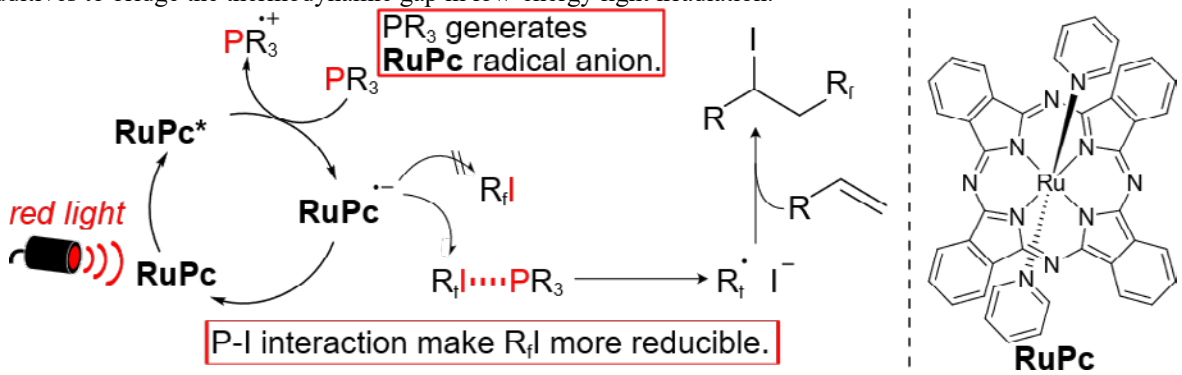
Ryo Nishida[a,b], Taniyuki Furuyama[b]

[a]*Graduate School of Medical Sciences, Kanazawa University, Kakuma-machi, Kanazawa, 920-1192, Japan*
[b]*Graduate School of Engineering, University of Hyogo, 2167 Shosha, Himeji, 671-2280, Japan*

Photoreactions driven by visible light have attracted significant attention for their ability to access unique chemical species unavailable through conventional thermal processes. While our group has developed various reactions utilizing long-wavelength light,[1] the use of low-energy red light often faces thermodynamic challenges, particularly in activating substrates with high reduction potentials. In this presentation, we report a red-light-driven iodoperfluoroalkylation of alkenes that overcomes these energy barriers by leveraging a unique synergistic effect between a perfluoroalkyl iodide (R_fI) and a phosphorus reagent.

Initially, we hypothesized that the reaction would proceed via a dual-catalyst system where ruthenium phthalocyanine (**RuPc**) acts as a red-light absorber and the phosphorus reagent serves as a substrate activator. Phosphorus reagents are known to interact with R_fI via phosphorus-iodine interactions, which can facilitate their reduction.[2] While **RuPc** successfully catalyzed the transformation under red-light irradiation in the presence of 1,4-bis(diphenylphosphino)butane (dppb), mechanistic investigations revealed a reaction mechanism different from the initial assumption. Spectroscopic and electrochemical analyses suggested that dppb plays an unexpected dual role in the catalytic cycle. Beyond activating R_fI through interatomic interactions, dppb also acts as a redox co-catalyst that undergoes reductive quenching with the excited **RuPc**. This quenching process generates a highly reactive **RuPc** radical anion, which possesses sufficient reducing power to activate the R_fI complex even under low-energy red-light excitation.

This reaction mechanism, combining substrate activation by phosphorus reagents with catalyst activation, enables efficient modification of various materials containing visible-light-absorbing dyes that were difficult to functionalize using conventional blue-light reactions due to competitive absorption. Our findings provide a new strategy on the design of red-light-driven catalytic systems by utilizing the unexpected redox-active properties of additives to bridge the thermodynamic gap in low-energy light irradiation.



REFERENCES

1. Furuyama *et al. J. Org. Chem.* **2024**, *89*, 8178; *Chem. Commun.* **2021**, *57*, 13594.
2. Czekelius *et al. Org. Lett.* **2019**, *21*, 7823.

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POSTERS



Can Strong-Light Matter Coupling Modify Potential Energy Surfaces?

Cora A. Noble[a], Thomas M. Khazanov[a], and Andrew J. Musser[a]

[a] *Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14853, USA*

Since their discovery, the hybrid states arising from strong light-matter coupling – known as exciton-polaritons – have gained attention in photochemistry due to their theoretical promise to reshape potential energy landscapes [1]. Polariton states are proposed to offer a transformative approach to materials engineering, for instance, providing a platform to modulate state energies and thereby photorelaxation processes such as internal conversion entirely non-synthetically, by simply incorporating molecules into an optical cavity. And yet, despite these expectations, there are many examples of exciton-polaritons in which strong coupling apparently induces negligible changes in photochemistry [2], or the changes can be explained by unrelated cavity-based effects [3]. The field thus currently faces a divide between exciting predictions of polariton-tuned dynamics and experimental observations of null results. In this work, we demonstrate with ultrafast spectroscopy that the internal conversion rate of certain benchmarking porphyrins, like Zinc (II) 5,10,15,20-tetraphenylporphyrin, can indeed be enhanced through strong light-matter coupling alone. We systematically evaluate the influence of key cavity structural parameters, including solid versus liquid environment, on the internal conversion rates of these porphyrins. Through this approach, we build crucial mechanistic insights and extract design principles that the field currently lacks. Beyond rewriting potential energy surfaces, the dynamics we study should profoundly impact how different excited states within strongly coupled cavities interact. Our design principles thus lay the groundwork to rationally enhance the performance of low-threshold organic polariton lasers, optical transistors, and other optical devices [4].

REFERENCES

1. Raphael F. Ribeiro, Luis A. Mart´ınez-Mart´ınez, Matthew Du, Jorge Campos-Gonzalez-Angulo, and Joel Yuen-Zhou. Polariton chemistry: controlling molecular dynamics with optical cavities. Chemical Science, 9(30):6325–6339, August 2018.
2. Dutta, A., Tiainen, V., Sokolovskii, I. et al. Thermal disorder prevents the suppression of ultra-fast photochemistry in the strong light-matter coupling regime. Nat Commun 15, 6600, 2024. https://doi.org/10.1038/s41467-024-50532-5
3. P. A.Thomas, W. J.Tan, V. G.Kravets, A. N.Grigorenko, W. L.Barnes. Non-Polaritonic Effects in Cavity-Modified Photochemistry. Adv. Mater., 36, 2309393, 2024. https://doi.org/10.1002/adma.202309393
4. Sanvitto, D.; Kéna-Cohen, S. The Road towards Polaritonic Devices. Nat. Mater., 15 (10), 1061–1073, 2016. https://doi.org/10.1038/nmat4668.

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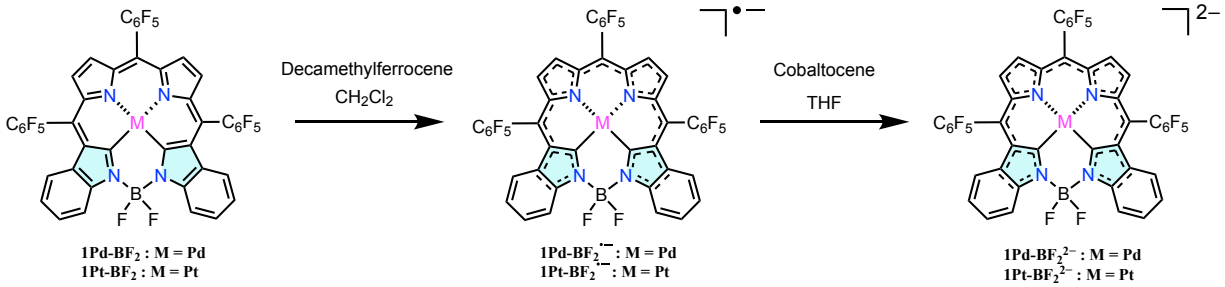


Redox-induced Aromaticity Switching in Doubly N-Confused Bilatriene Pd(II)/Pt(II) Complexes

Saori Okamura[a], **Masatoshi Ishida**[a]

[a]*Tokyo Metropolitan University Department of Chemistry, Graduate School of Science*

Redox-active dyes exhibit tunable optical properties upon electron transfer, enabling applications in sensors, chromic materials, bioimaging, and related fields. In particular, near-infrared (NIR)-absorbing dyes possess narrow HOMO–LUMO energy gaps that facilitate facile redox interconversion, a feature that is crucial for efficient molecular switching in biological probe applications. We previously reported novel open-chain tetrapyrrolic porphyrinoids, namely N-confused bilatriene [1] derivatives, that form Pt(II)- and Pd(II)-bridged organometallic species exhibiting strong NIR absorption arising from d_π–p_π interactions across the metal–carbon bond [2]. Furthermore, heterometallic complexes bearing a peripheral BF_2 unit (**1Pd-BF$_2$** and **1Pt-BF$_2$**) showed significantly lowered LUMO energy levels, enabling the formation of stable one- and two-electron reduced species (Scheme 1).



Scheme 1. Stepwise chemical reduction of **1Pd-BF$_2$** and **1Pt-BF$_2$**.

In this study, we successfully isolated and characterized the one-electron-reduced species (**1Pd-BF$_2$**$^{\bullet-}$ and **1Pt-BF$_2$**$^{\bullet-}$) and the two-electron-reduced species (**1Pd-BF$_2$**$^{2-}$ and **1Pt-BF$_2$**$^{2-}$) using chemical reductants such as decamethylferrocene and cobaltocene. Spectroscopic analyses revealed a characteristic low-energy absorption band around 1500 nm for **1Pt-BF$_2$**$^{\bullet-}$, which originates from its open-shell radicaloid electronic structure. In contrast, the two-electron-reduced species **1Pt-BF$_2$**$^{2-}$ displayed porphyrin-like sharp Soret and Q bands in the visible region, indicative of an aromatic electronic structure.

In the ^{1}H NMR spectra, the β-pyrrolic protons of **1Pt-BF$_2$**$^{2-}$ exhibited a notable downfield shift to δ = 7–8 ppm compared to those of the neutral complex **1Pt-BF$_2$** ($\delta_{\beta\text{-H}}$ = 5–6 ppm). The Pd congeners showed similar trends upon reduction, although the spectral shifts in both absorption and NMR were somewhat smaller than those observed for the Pt analogues. Finally, we evaluated the aromatic character and possible metallaaromaticity mediated by the bridging metal centers through theoretical calculations. Detailed structural features and spectroscopic properties will be discussed in this presentation.

REFERENCES

1. H. Furuta, M. Ishida *et al., ChemPlusChem* **2025**, *90*, e202500090.
2. J. Kim, M. Ishida, H. Furuta *et al., Angew. Chem. Int. Ed.* **2024**, *63,* e202405059.

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Post-Synthetic Diversification of BOPPY Fluorophores *via* Cross-Coupling and Nucleophilic Substitution Strategies

Sebastian O. Oloo[a], Petia Bobadova-Parvanova [b], Alexis A. Lueders[b], Mina Kim[b], Frank R. Fronczek[a], Kevin M. Smith[a], and Maria da Graça H. Vicente[a]

[a]*Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803*
[b]*Department of Chemistry and Fermentation Sciences, Appalachian State University, Boone, NC 28608*

BOPPY fluorophores, bis-BF_2-stabilized analogues of BODIPY dyes, remain underexplored as platforms for regioselective functionalization [1]. We report the selective halogenation of BOPPY followed by Pd-catalyzed cross-coupling and nucleophilic aromatic substitution to enable systematic diversification. Regioselective mono- and tri-bromination afforded versatile intermediates for Suzuki–Miyaura and Stille couplings, enabling efficient C–C bond formation with diverse aryl and heteroaryl partners. Nucleophilic substitution provided access to sulfur-substituted derivatives. Distinct regioselectivity was observed depending on the reaction pathway: Pd-catalyzed coupling of tribrominated BOPPY occurred preferentially at the β-position, whereas nucleophilic substitution favored the α-position. Computational studies supported the observed selectivity trends. These results establish halogenated BOPPY dyes as useful intermediates and provide a general strategy for their regioselective synthetic diversification.

REFERENCES

1. Yu, C.; Sun, Y.; Jiao, L.; Hao, E. Recent Advances in Highly Fluorescent Hydrazine-Inserted Pyrrole-Based Diboron-Anchoring Fluorophores: Synthesis and Properties. *Synlett* **2023**, a-2045-2369. https://doi.org/10.1055/a-2045-2369.

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Synthesis of Triangular Porphyrin Oligomers toward the Construction of Supramolecular Graphene

Oto Ooyama,[a] Yuki Shibata,[b] Ken-ichi Yamashita,[a,c] Shohei Saito[a]

[a] *Graduate School of Science, The University of Osaka. Japan*
[b] *Graduate School of Science, Kyoto University. Japan/*
[c] *ICS-OTRI, The University of Osaka. Japan*

By replacing the sp^2 carbon in graphene with a single triangular molecule and arranging these molecules such that their edges strongly interact, the resulting 2D nanosheet is expected to show an electronic band structure similar to that of graphene.[1] However, with reported triangular molecules designed for edge-to-edge interaction, such sheet-like structures have not yet been realized due to steric hindrance at the vertices.[2, 3] In this study, we designed and successfully synthesized triangular molecules in which cyclooctatetraene (COT) units are placed at the vertices and porphyrins are incorporated along the edges (Fig. 1). Construction of the nanosheet through formation of double-decker porphyrin complexes based on this triangular molecule has been tried. We will focus on the synthesis of the triangular and polygonal molecules, as well as preliminary investigations into their metal complexation.

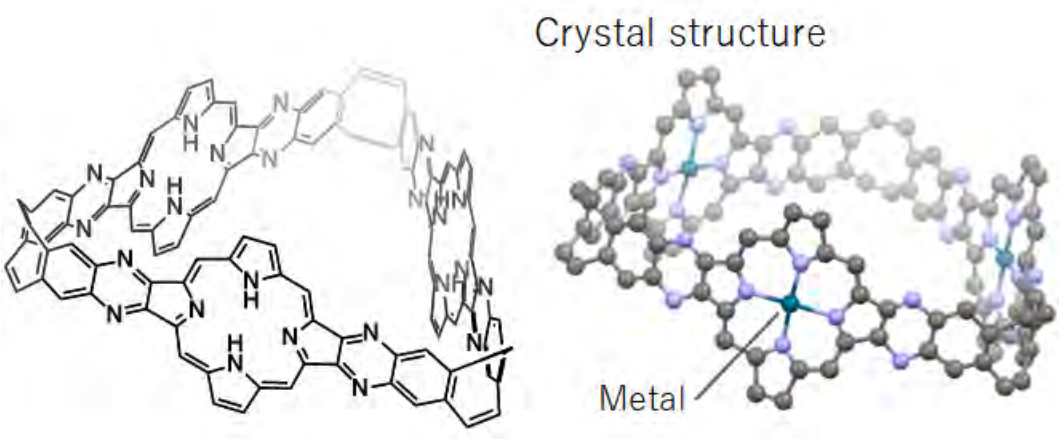


Figure 1. Molecular structure of the triangular molecule. (Substituents were omitted for clarity)

REFERENCES

1. K. Asano, and C. Hotta, *Phys. Rev*, *B* **2011**, *83*, 245125.
2. A. Mizuno, Y. Shuku, R. Suizu, M. M. Matsushita, M. Tsuchiizu, D. R. Mañeru, F. Illas, V. Robert, and K. Awaga, *J. Am. Chem. Soc*. **2015**, *137*, 7612.
3. Y. Beldjoudi, A. Narayanan, I. Roy, T. J. Pearson, M. M. Cetin, M. T. Nguyen, M. D. Krzyaniak, F. M. Alsubaie, M. R. Wasielewski, S. I. Stupp, and J. F. Stoddart, *J. Am. Chem. Soc*. **2019**, *141*, 17783.

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Influence of Surface Functionalization of Silicon Oxide Microchips on Cytocompatibility and Cellular Internalization

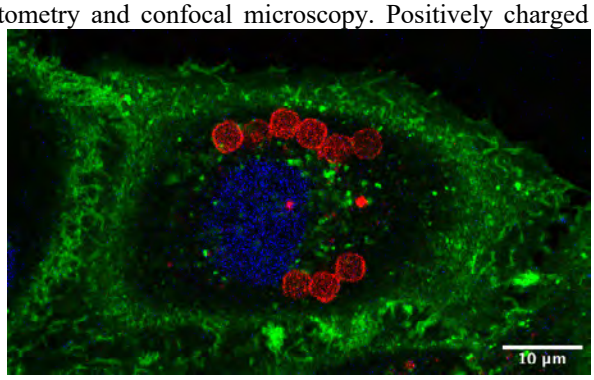
Pascual López-Algarra[a], Saman Bagherpour[a,b], Marta Duch[c], José Antonio Plaza[c], Josefa Badia[d], Laura Baldomà[d], Sergio Martínez-Ruiz[d], Lluïsa Pérez-García[a,b]

[a]*Departament de Farmacologia, Toxicologia i Química Terapèutica, Facultat de Farmàcia i Ciències de l'Alimentació, Univesitat de Barcelona, Barcelona, 08028, Spain. Email: mlperez@ub.edu*
[b]*Institut de Nanociència i Nanotecnologia IN2UB, Universitat de Barcelona, Barcelona, 08028, Spain.*
[c]*Instituto de Microelectrónica de Brcelona, IMB-CNM (CSIC), Campus UAB, Cerdanyola del Vallès, Barcelona, 08193, Spain.*
[d]*Departament de Bioquímica i Fisiologia, Facultat de Farmàcia i Ciències de l'Aalimentació, Universitat de Barcelona, 08028, Spain.*

POSTERS

Micrometric devices have attracted increasing attention for biomedical applications.[1] However, despite their biocompatibility and tunable surface chemistry, they often exhibit limited cellular uptake [2,3]. Self-assembled monolayers represent a reliable approach for modifying the surface chemistry of nano- and micromaterials. In this work, silicon oxide microchips (SiOμC) were functionalized with various silane derivatives to generate surfaces with different charge and wettability. Additionally, fluorescent labeling was added and enabled characterization and *in vitro* tracking.

Successful and stable modification was confirmed by water contact angle measurements and fluorescence imaging. Cytocompatibility was evaluated in HeLa and HaCaT cells, showing overall biocompatibility. Cellular association and internalization were assessed by flow cytometry and confocal microscopy. Positively charged SiOμC achieved the most efficient internalization, with up to 90% of HeLa cells containing internalized microchips at higher cell-to-chip ratios. These results highlight the critical role of surface chemistry in enabling cellular uptake of micrometer-sized silicon oxide microchips for biomedical applications.



Acknowledgments
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REFERENCES

1. Janjua, T. I.; Cao, Y.; Kleitz, F.; Linden, M.; Yu, C.; Popat, A. Silica Nanoparticles: A Review of Their Safety and Current Strategies to Overcome Biological Barriers. Adv Drug Deliv Rev 2023, 203, 115115.
2. Bruce, G.; Bagherpour, S.; Duch, M.; Plaza, J. A.; Stolnik, S.; Pérez-García, L. Exploring the Influence of Silicon Oxide Microchips Shape on Cellular Uptake Using Imaging Flow Cytometry. Microchimica Acta 2024, 191, 554.
3. Bagherpour, S.; Vázquez, P.; Duch, M.; Pablo Agusil, J.; Plaza, J. A.; Redondo-Horcajo, M.; Suárez, T.; Pérez-García, L. Silicon Oxide Microchips Functionalized with Fluorescent Probes for Quantitative Real-Time Glutathione Sensing in Living Cells. J Mater Chem B 2024, 13, 1630-1642.

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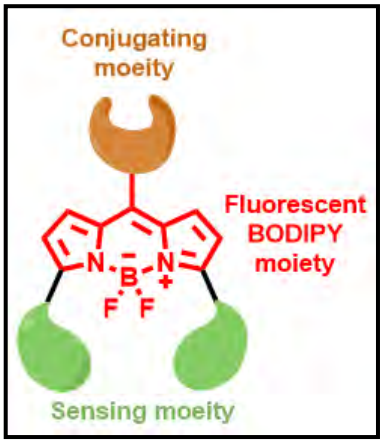


Mitochondria-Targeted BODIPY Fluorophores for Selective Sensing of Glutathione and Chloride Ion Dynamics

Ruxin Li[a,b], Sharanabasava D Hiremath[a,b], Saman Bagherpour[a,b] and Lluïsa Pérez-García[a,b]

[a]*Departament de Farmacologia Toxicologia i Química Terapèutica Universitat de Barcelona Av. Joan XXIII 27-31, Barcelona 08028, Spain. Email: mlperez@ub.edu*
[b]*Institut de Nanociència i Nanotecnologia IN2UB, Universitat de Barcelona, Barcelona, 08028 Spain*

Mitochondrial redox imbalance and ion dysregulation are closely associated with cancer progression, metabolic reprogramming, and therapeutic resistance. Elevated glutathione (GSH) levels serve as cancer biomarkers, while mitochondrial chloride (Cl^-) homeostasis modulates redox potential and apoptotic signalling [1]. Herein, we report two structurally related BODIPY-based fluorescent probes for selective mitochondrial sensing of GSH and chloride ion channels via distinct recognition mechanisms.



Both probes incorporate a terminal alkyne as a bioorthogonal handle for mitochondrial targeting. The GSH probe contains an electron-withdrawing diethyl malonate moiety, enabling reversible Michael addition with GSH for real-time monitoring of mitochondrial redox adaptation [2]. The chloride probe features a pyrrole-linked benzimidazolyl hydrazone unit that selectively binds Cl^- through directional hydrogen bonding and self-assembles into nanochannels, facilitating HCl translocation across lipid bilayers [3].

Overall, this modular BODIPY strategy provides complementary tools for investigating mitochondrial redox and ionic dysregulation in cancer-relevant systems.

ACKNOWLEDGMENTS

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REFERENCES

1. (a) J. T. Davis, P. A. Gale, R. Quesada, *Chem. Soc. Rev*. **2020**, *49*, 6056–6086; (b) C. R. Bartman, D. R. Weilandt, Y. Shen, W. D. Lee, Y. Han, T. TeSlaa, C. S. R. Jankowski, L. Samarah, N. R. Park, V. da Silva-Diz, et al., *Nature* **2023**, *614*, 349–357.
2. (a) R. Kumar, S. Sandhu, P. Singh, S. Kumar, *Chem. Rec*. **2017**, *17*, 441–471 ; (b) Z. Xu, S. K. Kim, J. Yoon, *Chem. Soc. Rev*. **2010**, *39*, 1457–1466.
3. (a) P. A. Gale, J. T. Davis, R. Quesada, *Chem. Soc. Rev*. **2017**, *46*, 2497–2519; (b) J. T. Davis, O. Okunola, R. Quesada, *Chem. Soc. Rev*. **2010**, *39*, 3843–3862.

POSTERS

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Arsenic Corroles

Hendrik Peters,[a] **Martin Bröring**[a]

[a]*IAAC, TU Braunschweig, Germany.*

Corrole macrocycles have aroused research interest as part of porphyrinoid chemistry. Due to the tri-ionic nature, coordinated metals are stabilized in high oxidation states. Thus, a whole variety of metal corroles have been reported.[1] Despite this, publications on main group corroles remain few and far between, especially for the 5th main group.[2, 3]
Kadish published As, Sb and Bi corroles with oxidation states of +3, +4 and +5.[4] Since then, no further reports have been published on arsenic corroles, which might correlate with the toxic starting material $AsCl_3$ for this synthesis. Hence, less-toxic material was used as the new starting reagent for arsenic corroles bearing different functional groups. Furthermore, new synthetic routes were established to yield arsenic corroles in formal oxidation states of +4 and +5 with different axial ligands and will be presented on the poster.

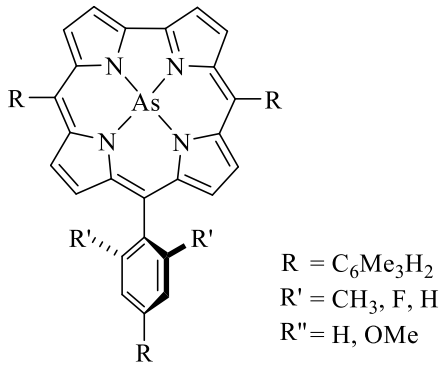


Figure 1. Arsenic corroles with oxidation state of +3

REFERENCES

[1] J. F. B. Barata, M. G. P. M. S. Neves, M. A. F. Faustino, A. C. Tomé, J. A. S. Cavaleiro, *Chem. Rev.* **2017**, 117, 3192–3253.
[2] S. Eulberg, N. Schulze, J. Krumsieck, N. Klein, M. Bröring, *Angew. Chem.* **2023**, 135.
[3] L. M. Reith, M. Stiftinger, U. Monkowius, G. Knör, W. Schoefberger, *Inorg. Chem.* **2011**, 50, 6788–6797.
[4] K. M. Kadish, C. Erben, Z. Ou, V. A. Adamian, S. Will, E. Vogel, *Inorg. Chem.* **2000**, 39, 3312-3319.

POSTERS

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Visible- and UV-Raman Spectroscopy of Nitric Oxide Reductase and Heme-Copper Oxidase Reactions with NO

Eftychia Pinakoulaki[a], Takehiro Ohta[b], Teizo Kitagawa[b],Tewfik Soulimane[c], Constantinos Varotsis[d]

[a]*Department of Chemistry, University of Cyprus, 2109 Aglantzia, Cyprus*
[b]*Okazaki Institute for Integrative Bioscience, National Institutes of Natural Sciences 5-1 Higashiyama, Myodaiji, Okazaki, Aichi 444-8787 Japan*
[c]*University of Limerick, Limerick, Ireland*
[d]*Department of Chemical Engineering Cyprus,University of Technology, Limassol, Cyprus*

In bacterial respiration the reduction of NO to N_2O by terminal oxidases supports the hypothesis of a common evolutionary origin of bacterial denitrification and aerobic respiration. Activation of NO in denitrification and bacterial respiration provides the means to identify conserved structural features, which can be assumed to be involved in basic functions common to both classes. Elucidation of the structures and the electronic configurations of intermediates are of profound importance for understanding the mechanism by which the enzymes form and cleave NO-containing bonds. [1-6] The formation of the hyponitrite species from two NO molecules is the key intermediate in the reduction of NO. Visible and UV-Raman studies of the NO structures formed in the heme Fe-Cu_B and Heme Fe-Fe centers will be presented.

REFERENCES

1. Koutsoupakis, C.; Soulimane, T.; Varotsis, C. Discrete Ligand Binding and Electron Transfer Properties of *ba*$_3$-Cytochrome *c* Oxidase from *Thermus thermophilus*: Evolutionary Adaption to Low Oxygen and High Temperature Environments**.** *Acc. Chem. Res.* **2019**, *52* (5), 1380-139.
2. Loullis, A.; Noor, M.R.; Soulimane, T.; Pinakoulaki, E. The structure of a ferrous heme-nitro species in the binuclear heme a_3/Cu_B center of *ba*$_3$-cytochrome *c* oxidase as determined by resonance Raman spectroscopy. *Chem. Commun.* **2015**, *51* (2), 286-289.
3. Varotsis, C.; Ohta, T.; Kitagawa, T.; Soulimane, T.; Pinakoulaki, E. The Structure of the Hyponitrite Species in a Heme Fe-Cu Binuclear Center. *Angew. Chem. Int.* **2007**, *46*, 2210-2214.
4. Ohta, T.; Kitagawa, T.; Varotsis, C. Characterization of a Bimetallic-Bridging Intermediate in the Reduction of NO to N_2O: a Density Functional Theory Study. *Inorg. Chem.* **2006**, *45*, 3187-3190.
5. Ohta, T.; Soulimane, T.; Kitagawa, T.; Varotsis, C. Nitric oxide activation by *caa*$_3$ oxidoreductase from *Thermus thermophilus*. *Phys. Chem. Chem. Phys.* **2015**, *17* (16), 10894-1089.
6. Daskalakis, V.; Ohta, T.; Kitagawa, T.; Varotsis, C. Structure and properties of the catalytic site of nitric oxide reductase at ambient temperature. *Biochim. Biophys. Acta -Bioenerg.* **2015**, *1847* (10), 1240.

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Resonance Raman and FTIR Investigation of the Reactions of Hemeproteins with Sulfide/Nitrite

Eftychia Pinakoulaki, and Vasiliki Valianti

Department of Chemistry, University of Cyprus, 2109 Aglantzia, Cyprus

Myoglobin (Mb) and hemoglobin (Hb), associated with oxygen transport and storage, are now also considered to be actively involved in signaling pathways. These hemeproteins can function as nitrite reductases (NiRs) converting nitrite (NO_2^-) to nitric oxide (NO) during metabolic stress and hypoxic conditions, and potentially serve as sulfide oxidases for hydrogen sulfide (H_2S) detoxification. Although the coordination and redox chemistry of NO_2^- and H_2S with the hemeproteins have been investigated independently [1-4], data for heme-mediated H_2S/NO_2^- crosstalk are lacking. In this work, resonance Raman and FTIR spectroscopies have been employed to investigate the redox reactions of Mb and Hb in the presence of both substrates (H_2S/NO_2^-). The vibrational characterization of the species formed in the heme Fe center of Mb and Hb will be presented and discussed.

REFERENCES

1. Valianti, V. K., Tselios, C., Pinakoulaki, E., Reversible thermally induced spin crossover in the myoglobin–nitrito adduct directly monitored by resonance Raman spectroscopy. *RSC Adv.* (2023) 13, 9020-90252.
2. Ioannou, A., Lambrou, A., Daskalakis, V., Pinakoulaki, E. Nitrite Coordination in Myoglobin. *J. Inorg. Biochem.* (2017) 166, 49–54.
3. Lambrou, A., Pinakoulaki, E. Resonance Raman Detection of the Myoglobin Nitrito Heme Fe-O-N=O/2-Nitrovinyl Species: Implications for Helix E-Helix F Interactions. *Phys. Chem. Chem. Phys.* (2015) 17, 3841-3849.
4. Palermo, J. C., Carllinni Colombo, M., Semelak, J. A., Scocozza, M. F., Boubeta, F. M., Murgida, D. H., Estrin, D. A., Bari, S. E. Autocatalytic Mechanism in the Anaerobic Reduction of Metmyoglobin by Sulfide Species. *Inorg. Chem.* (2023) 62, 11304–11317.

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A Cobalamin-Dependent Radical SAM Methyltransferase that Methylates SAM – Characterization and Exploration of the Alkyl-Transfer Potential of Orf29

Fabian Piskol[a], **Gunhild Layer**[a]

[a] *Albert-Ludwigs-Universität Freiburg, Institute of Pharmaceutical Sciences, Stefan-Meier-Str. 19, 79104 Freiburg i. Br., Germany*

The unusual cyclopropane-containing amino acid (1*S*,2*S*)-2-methyl-1-aminocyclopropane-1-carboxylic acid ((1*S*,2*S*)-MeACC) is biosynthesized in a two-step enzymatic process that utilizes *S*-adenosyl-L-methionine (SAM) as initial substrate. In the first step, a cobalamin-dependent radical SAM methyltransferase (B12-RSMT), termed Orf29, catalyzes the methylation of the methionine moiety of SAM yielding (4″*R*)-4″-methyl-SAM [1]. Second, a cyclization reaction leads to the formation of (1*S*,2*S*)-MeACC [1]. This product serves as a building block for natural products exhibiting antibiotic and/or antitumor activities [2-3].

The putative B12-RSMT Orf29 from *Streptomyces coffeae* (*Sc*) was characterized as a homo-dimer which contains one [4Fe-4S]-cluster and one cobalamin (Cbl) in base-off conformation per subunit. LC-MS analysis of *in vitro* enzymevactivity assays of *Sc*Orf29 revealed the methylation of SAM to methyl-SAM. The formation of 5′-deoxyadenosine (5'-dA) and *S*-adenosyl-L-homocysteine (SAH) was observed by HPLC analysis in an approx. 1:1 ratio and the enzyme followed a typical B12-RSMT mechanism [4]. Next, we investigated binding promiscuity, affinities and the alkyl-transfer potential of *Sc*Orf29 using different alkyl-cobalamins prepared as described in the literature [5]. The respective alkyl-cobalamins were bound in the enzyme and the transfer of different alkyl-groups was catalyzed by *Sc*Orf29. Additionally, structure analysis by cryogenic electron microscopy confirmed the base-off conformation of the cobalamin co-factor and the obtained structure of *Sc*Orf29 allows for the elucidation of how this enzyme utilizes three molecules of SAM as substrate, co-factor and methyl-group donor during catalysis.

We acknowledge funding by Deutsche Forschungsgemeinschaft (DFG) of FOR project 510974120.

REFERENCES

1. Maruyama et al., *Biomolecules* 2020, 10 (5), 775. DOI: 10.3390/biom10050775.
2. Kurosawa et al., *J. Antibiot.* 2001, 54 (8), 615–621. DOI: 10.7164/antibiotics.54.615.
3. Nakaya et al., *Biosci. Biotechnol. Biochem.* 2007, 71 (12), 2969–2976. DOI: 10.1271/bbb.70371.
4. Gagsteiger et al., *Angew. Chemie Int. Ed.* 2022, 61 (32), e202204198. DOI: 10.1002/anie.202204198.
5. Hannibal et al., *Inorg. Chem.* 2009, 48 (14), 6615–6622. DOI:10.1021/ic900590p.

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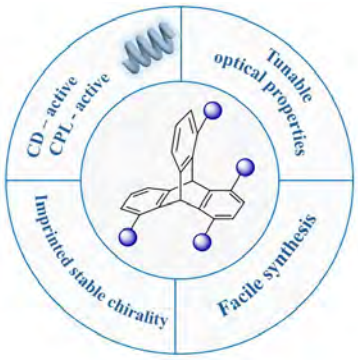


Chiroptically active 3D macrocycles based on triptycene

Sonia Polańska[a], Krzysztof Dzieszkowski[a], Ludovic Favereau[b], Miłosz Pawlicki[a]

[a]Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland
[b]University of Rennes, CNRS, ISCR– UMR 6226, ScanMAT– UMS 2001, F-35000 Rennes, France

The π-extended and fully organic and aromatic chromophores are driving advances across material science due to their highly efficient light absorption and emission. Recently, the chirality within strongly conjugated structures was mostly incorporated by the formation of helical structures [1] and the class of macrocyclic systems bearing a figure-eight conformation [2]. The rapid development of high-performance chiroptical materials creates the necessity of looking for structures more capable toward low energetic absorbance and effective luminescence, including a specific behaviour in polarized light.



Despite intensive research, the chiral material exhibiting synergistic enhancement of g_{abs}/g_{lum} values, quantum yield, with a combination of straightforward synthesis and effective chiral separation has yet to be achieved [3]. Currently, systematic studies to determine the structural factors responsible for efficient absorption and emission in polarized light in a wide range of chiral macrocycles are in their infancy.

Herein, we report the synthesis and chiroptical properties of a novel functional organic chromophore based on a rigid triptycene core decorated with macrocyclic loops. The developed structure belongs to a novel class of hybrid optic materials showing extraordinary absorbance and fluorescence capable of playing an important role in tuning the optical properties, in addition to imprinted stable chirality.

REFERENCES

1. Shen, Y. et al. *Chem. Rev.* **2012**, 112, 1463-1535.
2. Klajn, J. et al. *Chem. Commun.* **2019**, 55, 4558−4561.
3. Xu, Q. et al. *Adv. Optical Mater.* **2025**, 13, e01569.

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Tuning Cytotoxic Properties of Phosphorus(V) Porphyrins for Biomedical Applications

Marina A. Polovkova[a], Inessa A. Efimova[a], Evgeniya A. Safonova[a], Roman A. Akasov[b], Aslan Yu. Tsivadze[a,c], Yulia G. Gorbunova[a,c,d]

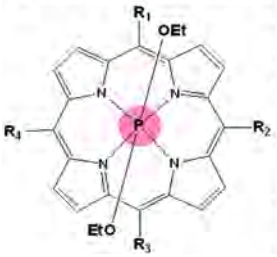
[a] *Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, Moscow, Russia*
[b] *Institute of Molecular Theranostics, Sechenov First Moscow State Medical University, Moscow, Russia*
[c] *Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, Moscow, Russia*
[d] *Faculty of Fundamental Physical and Chemical Engineering, Lomonosov Moscow State University, Moscow, Russia*

The search for new, more efficient photosensitizers that are highly cytotoxic, rapidly eliminated, and water-soluble remains high in demand. Previously, it was shown that introducing a P(V) atom into the porphyrin macrocycle leads to the formation of water-soluble cationic complexes. The presence of axial ligands at the P(V) atom prevents aggregation and also allows the photophysical and photochemical properties of these compounds to be tuned. Additionally, it has been confirmed that P(V) porphyrins can effectively generate singlet oxygen in aqueous media, making these compounds promising photosensitizers [1].

Here, we present a series of P(V) porphyrins, demonstrating the influence of meso-substituent and axial-ligand nature on cytotoxic properties. Complexes containing axial –OEt groups were found to exhibit nanomolar and picomolar phototoxicity against A-549 lung adenocarcinoma cells and MCF-7 breast adenocarcinoma cells when irradiated with 450 nm light. It was shown that **1**, **2** and **5** ($IC_{50\ light}$ = 14, 9, and 15 nM, respectively) exhibit the highest light toxicity against MCF-7 cells, with **5** having the highest phototoxicity index (PI = 60.2), whereas for **1** and **2**, PI=3.2 and 4.7, respectively. Moreover, the **5** demonstrated a record light toxicity value against A-549 cells, with a toxicity value of 330 pM, and the highest PI = 153. Thus, **1**, **2**, **4**, and **5** are the most photocytotoxic compounds with nanomolar phototoxicity and are promising for use as photosensitizers.

For the first time, it was demonstrated that complexes **4** and **5** with electron-donating meso-substituents exhibit nanomolar light toxicity ($IC_{50\ light}$ = 6.4 - 14.5 nM) when irradiated with 660 nm light in both cell lines. This is the first example of the photocytotoxic effect of P(V) porphyrins when irradiated within the therapeutic window of tissue transparency.

Dark and light cytotoxicity of P(V) porphyrins against MCF-7 and A-549 cells.



Compound	MCF-7			A-549		
	$IC_{50\ dark}$, nM	$IC_{50\ light\ 450}$, nM	PI	$IC_{50\ dark}$, nM	$IC_{50\ light\ 450}$, nM	PI
(1) R_1=R_2=R_3=R_4=Ph	45	14.0	3.2	46	5.7	8.1
(2) R_1=R_2=R_3=Ph, R_4=Py	42	8.9	4.7	129	2.0	64.5
(3) R_1=R_3=Ph, R_2=R_4=Py	100	92	1.1	265	35	7.6
(4) R_1=R_2=R_3=R_4=PhMe	863	170	5.1	50.5	18.5	10.9
(5) R_1=R_2=R_3=R_4=PhOMe	903	15	60.2	201.1	0.33	153
Compound	$IC_{50\ dark}$, нМ [1]	$IC_{50\ light\ 660}$, нМ [3]	PI	$IC_{50\ dark}$, нМ [1]	$IC_{50\ light\ 660}$, нМ [3]	PI
(4) R_1=R_2=R_3=R_4=PhMe	863	11.3	76.4	50.5	6.5	30.9
(5) R_1=R_2=R_3=R_4=PhOMe	903	14.5	62.3	201.1	6.4	7.9

Acknowledgement: This work was supported by the Russian Science Foundation (grant № 24-73-10192).

REFERENCES

1. I.A. Efimova et al., *Dalt. Trans.* **2025**, 54(24), 9553–9564.

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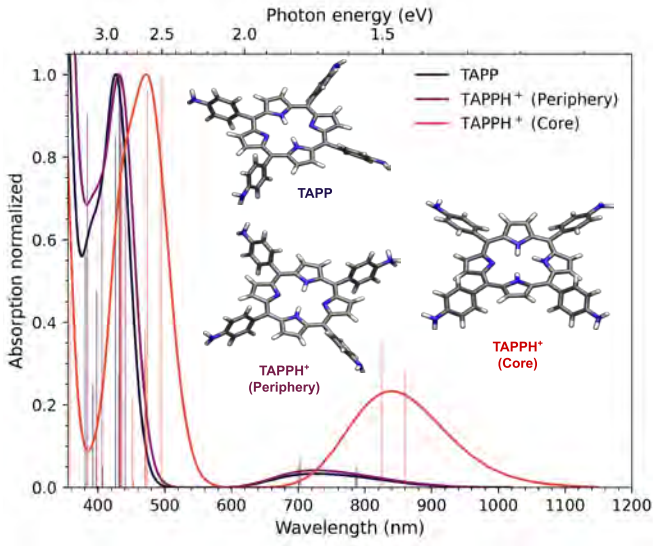
First-Principles Analysis of Protonation-Induced Electronic Effects in Tetrakis(*p*-aminophenyl)porphyrin (TAPP)

Arghyadeb Roy[a,b,f], Anna Elmanova[a,f], Sujith Jayan[a], Maximilian L. Hupfer[a], Todd J. Martínez[c,d], Daniel T. Gryko[b], Martin Presselt[a,e,f]

[a] *Leibniz Institute of Photonic Technology (IPHT), Jena, Germany*
[b] *Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52,01-224 Warsaw, Poland*
[c] *Department of Chemistry and the PULSE Institute, Stanford University, Stanford, California 94305, USA*
[d] *SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA*
[e] *Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany*
[f] *Sciclus GmbH & Co. KG, Moritz-von-Rohr-Str. 1a, 07745 Jena, Germany*

Porphyrins exhibit electronic and optical properties that are highly sensitive to protonation [1]. We present a first-principles density functional theory study of neutral and protonated porphyrins [2], focusing on geometry relaxation, electronic structure, and changes in UV–vis spectra. Core protonation induces symmetry breaking and charge redistribution, leading to characteristic Q-band shifts consistent with experimental results [3–4], while peripheral protonation preserves variant symmetry and produces distinct spectral signatures.

These results identify protonation as an effective molecular handle for tuning porphyrin photophysics, thus establishing a comprehensive picture of how local chemical changes govern porphyrin optical response in functional materials.



REFERENCES

1. W. Beenken, W. Maes, M. Kruk, T. Martínez, M. Presselt, *J. Phys. Chem. A* 2015, *119* (26), 6875-6883
2. M. Presselt, W. Dehaen, W. Maes, A. Klamt, T. Martínez, W. J. D. Beenken, M. Kruk, *Phys. Chem. Chem. Phys*. 2015, *17*, 14096–14106.
3. J. R. Weinkauf, S. W. Cooper, A. Schweiger, C. C. Wamser, *J. Phys. Chem. A* 2003, *107* (18), 3486–3496
4. C. Wang, C. C. Wamser, *J. Phys. Chem. A* 2014, *118* (20), 3605–3615

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Ab-initio Mapping of π-Stacking Motifs in 5,10,15,20-Tetrakis(4-aminophenyl)porphyrin (TAPP): From Dimer Landscapes to Extended Aggregates

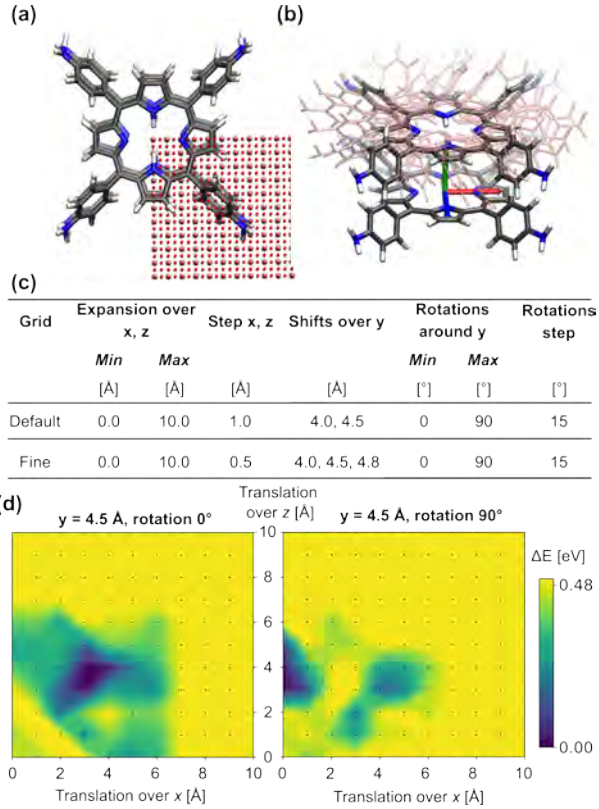
Anna Elmanova[abc], Arghyadeb Roy[ad], Maximilian L. Hupfer[a], Martin Presselt[a,d]

[a] *Leibniz Institute of Photonic Technology (IPHT), Jena, Germany*
[b] *Institute of Physical Chemistry, Friedrich Schiller University Jena, Helmholtzweg 4, 07743 Jena, Germany*
[c] *SciClus GmbH&Co. KG, Moritz-von-Rohr-Str. 1a, 07745 Jena, Germany*
[d] *Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52,01-224 Warsaw, Poland*
[e] *Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany*

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π–π interactions govern the supramolecular structure and functionality of π-conjugated semiconductor materials, yet predicting aggregate geometries remains challenging due to the vast configurational space[1].

Building on our previously established DFT-based framework for systematic prediction of porphyrin π-stacks[2], we extend this methodology to investigate aggregation of 5,10,15,20-tetrakis(4-aminophenyl)porphyrin (TAPP). Systematically varied dimer geometries are generated using structured translational and rotational grids (Figure 1, panels a,b,c). Single-point DFT calculations identify local energy minima (sample landscapes shown in Figure 1d). Energetically favorable representatives of clustered dimer families are optimized and subsequently propagated to larger aggregates. This also provides a transferable strategy for studying π-conjugated covalent organic networks built from TAPP building blocks.



Grid	Expansion over x, z		Step x, z	Shifts over y	Rotations around y		Rotations step
	Min	*Max*			*Min*	*Max*	
	[Å]	[Å]	[Å]	[Å]	[°]	[°]	[°]
Default	0.0	10.0	1.0	4.0, 4.5	0	90	15
Fine	0.0	10.0	0.5	4.0, 4.5, 4.8	0	90	15

Figure 1. Grids used to determine dimers of TAPP and corresponding energy landscapes. Panel (a): Default spatial grid (pink markers) with fine grid (red markers). Panel (b): Rotational grid with step around y axis of 15°. Panel (c): Details of the grids used. Panel (d) : Sample energy landscapes for two selected rotations.

REFERENCES

1. T. Sachse, T. J. Martinez, B. Dietzek and M. Presselt, *J Comput Chem* **2018**, *39*, 763-772.
2. A. Elmanova, B. O. Jahn and M. Presselt, *J Phys Chem A* **2024**, *128*, 9917-9926.

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Inducing Helical Handedness in π-Extended Macrocycles via Axial Chirality Transfer

SK J. Rahaman[a], K. Dzieszkowski[a], M. Kijewska[b],L. Favereaue[c], M. Pawlicki[a]*

[a] *Faculty of Chemistry, Jagiellonian University,30-387 Krakow, Poland*
[b] *Department of Chemistry, University of Wroclaw, 50383 Wroclaw, Poland*
[c] *Department of Chemistry, University of Rennes, CNRS, ISCR– UMR 6226, ScanMAT– UMS 2001, F-35000 Rennes, France*

Since Pasteur first identified molecular chirality in 1848, the ability to control "handedness" has become vital for applications ranging from biological sensing to advanced optoelectronics. The integration of chirality into organic semiconductors enables powerful photonic and spintronic functionalities, including circularly polarized luminescence (CPL), chiral-induced spin selectivity (CISS) effect [1], and chiral redox-switchable materials. Despite their promise, the scalable deployment of chiral organic materials remains severely limited by the challenge of accessing enantiopure compounds, which typically relies on low-throughput and costly HPLC separations. Enforcing macrocyclization through the sterically encumbered 2,2′-positions imposes substantial torsional strain, rendering such architectures synthetically demanding and conceptually unexplored for the design of chiral materials.

Herein, we transform these inherent challenges into design opportunities by introducing an HPLC-free synthetic platform that exploits axial-to-helical chirality transfer to access a diverse family of enantiomerically enriched π-extended fluorophores. Central to this strategy is the design of a chirality-imprinted, novel macrocyclic architecture with finely controlled dynamicity. By locking the conjugation pathway, the macrocycles exhibit pronounced chiroptical responses, including strong circular dichroism (CD) and circularly polarized light (CPL). Conversely, unlocking the conjugation restores biaryl dynamicity, introducing open-shell character and adaptive electronic behaviour[2]. The study demonstrates that by modulating the π-extension, one can take a macrocyclic avenue to create redox-switchable materials[3]. We'll present the synthetic methodology and comprehensive spectroscopic investigation of three macrocyclic systems spanning distinct conjugation regimes, supported by theoretical calculations. This platform offers a scalable paradigm for designing dynamically tunable semiconductors for next-generation spintronic and photonic devices.



REFERENCES:

1. J.Q.Wang, X.N.Han, Y.Han, C.F.Chen, *Chem. Commun*., **2023**,59, 13089
2. P.Banachowicz, M.Das, K.Kruczała, M.Siczek, Z.Sojka, M.Kijewska, M.Pawlicki, *Angew. Chem. Int. Ed*. **2024**, 63, e202400780.
3. A.Dutta, K.Dzieszkowski, M.Kijewska, M.siczek, L.Orzel, M.Pawlicki, *Chem. Commun*., **2025**,61, 9424-9427

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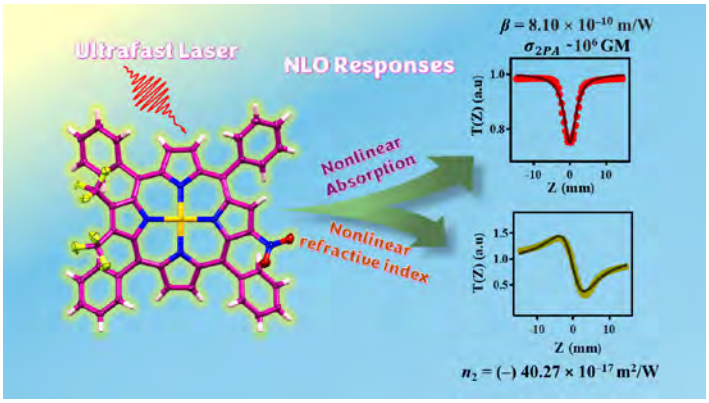


Structure-Driven Enhancement of Third-Order Nonlinear Optical Properties in Electron-Deficient *β*-Trisubstituted Porphyrins

Reena, and Muniappan Sankar*

Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 24667, India

The development of nonlinear optical (NLO) materials combining strong optical nonlinearity with high stability is critical for emerging photonic and optoelectronic applications.[1] Porphyrins are attractive NLO candidates owing to their highly delocalized aromatic π-electron systems, exceptional chemical stability, conformational flexibility, and amenability to structural modulation.[1] While unsymmetrical push-pull porphyrins have been extensively explored, electron-deficient unsymmetrical porphyrins remain largely unexplored due to their synthetic challenges. In this work, a new series of electron-deficient antipodal β-trisubstituted porphyrins, 12-nitro-5,10,15,20-tetraphenyl-2,3-bis(trifluoromethyl)porphyrin ($H_2TPP(NO_2)(CF_3)_2$) and its metal complexes, Co^{II}, Ni^{II}, Cu^{II}, and Zn^{II}, were successfully synthesized and comprehensively characterized using spectroscopic techniques and single-crystal X-ray diffraction.[1e] These unsymmetrical porphyrins exhibit intriguing photophysical and electrochemical properties arising from asymmetric electron-deficient *β*-substitution. Intensity-dependent third-order NLO measurements reveal pronounced two-photon absorption with coefficients (β) ranging from 0.04 to 8.10×10^{-10} m/W and cross-sections (σ_{2PA}) of 0.02-1.67 × 10^6 GM, along with strong self-defocusing behavior characterized by negative nonlinear refraction (n_2 = -1.08 to - 40.27 × 10^{-17} m^2/W).[1e] These findings establish electron-deficient unsymmetrical porphyrins as promising materials for advanced photonic and optoelectronic applications.[1e]



REFERENCES

1. (a) M. Samal *et al*. *Chem. Commun*., **2019**, *55*, 11025-11028. (b) M. Sankar *et al*. *Inorg. Chem.,* **2024**, *63*, 17967−17982. (c) A. S. Bulbul *et al*. *Inorg. Chem.,* **2022**, *61*, 9968−9982. (d) R. K. Rohal *et al*. *Dalton Trans*., **2024**, 53, 6436. (e) R. Jangra *et al*. *Dalton Trans.*, **2025**, *54*, 10234-10245.

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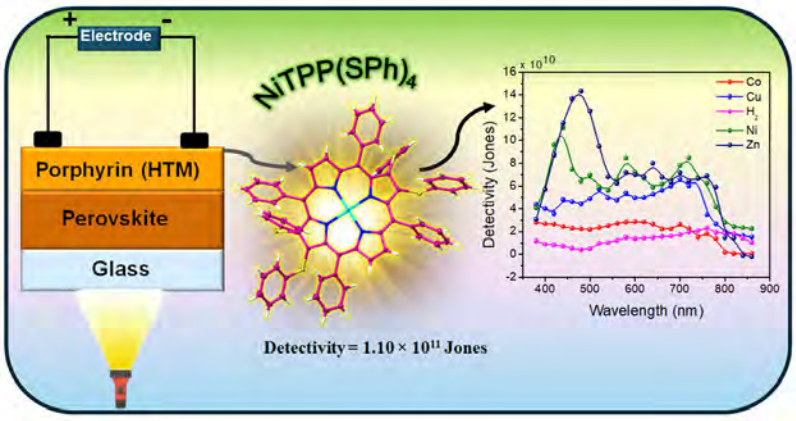
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Redox-Active β-Tetrathiophenols Porphyrins as Next-Generation Hole-Transport Materials in Perovskite Photodetectors

Reena, and Muniappan Sankar*

Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247667, India

Porphyrin-based hole-transporting materials, with tunable frontier orbital energies, extended π-conjugation, and structural versatility, offer efficient charge extraction while suppressing recombination losses.[1] Their incorporation into perovskite photodetectors has been shown to markedly enhance responsivity, detectivity, and operational stability, underscoring their promise as next-generation HTMs.[1] Here, we report a new class of highly nonplanar, *β*-tetrathiophenyl appended porphyrins, MTPP(SPh)$_4$ (M = 2H, Co^{II}, Ni^{II}, Cu^{II}, and Zn^{II}), and demonstrate their effectiveness as solution-processable hole-transport layers (HTLs**)** in lateral $FA_{0.9}Cs_{0.1}Pb(I_{0.94}Br_{0.06})_3$ perovskite photodetectors. Single-crystal X-ray diffraction and density functional theory calculations reveal a pronounced macrocyclic distortion induced by bulky *β*-thiophenyl substituents, resulting in elevated HOMO levels, reduced energy gaps, and enhanced redox activity. When incorporated at the perovskite interface, these nonplanar porphyrins significantly suppress dark current, reduce charge-transfer resistance, and enhance hole extraction, as confirmed by current-voltage analysis, impedance spectroscopy, and illumination-intensity-dependent measurements. Among the series, Ni- and Zn-porphyrin-based devices exhibit the best overall performance, delivering broadband photodetection across 400-720 nm with detectivities exceeding 10^{11} Jones and fast temporal response.[1e] This work establishes a clear structure-energetics-transport relationship and identifies controlled porphyrin nonplanarity combined with *β*-electron-donating substitution as a general molecular design strategy for high-performance perovskite photodetectors and related optoelectronic devices.[1e]



REFERENCES

1. (a) L. Xiao *et al*. *J. Mater. Chem. C,* **2018**, *6*, 3341. (b) M. Xie *et al*. *RSC Adv.*, **2023**, *13*, 24699. (c) L. Li *et al*. *J. Mater. Chem. C,* **2014**, *2*, 1372. (d) YB Tian *et al*. *Adv. Sci.,* **2021**, *8*, 2100548. (e) R. Jangra, A. Sengupta, B. Diwakar, M. A. Afroz, S. Satapathi and M. Sankar, *Manuscript Submitted for Publication*.

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Synthesis of Low-Symmetrical Silicon Phthalocyanines for Photodynamic Therapy

Leon David Rodrigues[a], Veronika. Novakova[a]

[a] *Department of Pharmaceutical Chemistry and Pharmaceutical Analysis, Faculty of Pharmacy in Hradec Králové, Charles University, Akademika Heyrovskeho 1203, Hradec Králové 50003, rodrigule@faf.cuni.cz*

Photodynamic therapy (PDT) is an effective cancer therapy that involves a photochemical reaction between a photosensitizer (PS), light, and molecular oxygen [1]. Phthalocyanines (Pcs), one of such PSs, are aromatic macrocycles having 18 π-electrons comprised of four isoindole units linked together through their 1,3-positions by aza bridges. Pcs have maximal absorption in the phototherapeutic window of tissues (i.e., 650-800 nm), and can produce high singlet oxygen, making them optimal PSs for PDT for cancer. The main drawback of clinically approved PSs is their accumulation in the body and subsequent skin photosensitivity. The solution could be the development of unique Pcs with more modifiable sites, enabling the introduction of a targeting moiety, a switchable group for in vivo activation, and a moiety that increases hydrophilicity within a single Pc molecule. Low-symmetrical silicon(IV) Pcs (SiPcs) may be promising candidates for that.

Therefore, we focused on developing a method to prepare low-symmetrical SiPc (Fig. 1) that can be functionalized at both the periphery and axial positions. Our method is based on the synthesis of low-symmetrical metal-free Pc followed by coordination of Si(IV) to the centre and introduction of axial ligands. Unexpectedly, we observed an interesting ring contraction as a side reaction. Conditions were studied in detail to describe the key parameters for the formation of contracted macrocycles and to maximise the yields of target SiPcs. Prepared derivatives were investigated from a spectral and photophysical perspective, and the most promising compound was further conjugated to an aptamer as a targeting moiety.

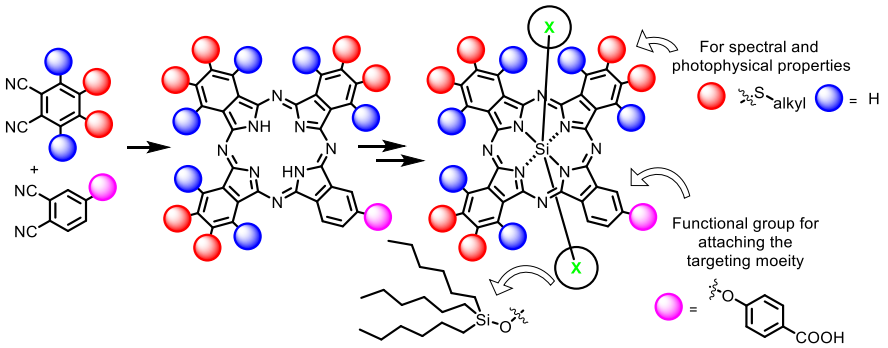


Figure 1. Developed a method for low-symmetrical SiPcs

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REFERENCES

1. Lo, P. C., Rodríguez-Morgade, M. S., Pandey, R. K., Ng, D. K., Torres, T., Dumoulin, F., Chem. Soc. Rev., 2020, 49, 1041.

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A Greener Route to Blue: Solid-State Synthesis and Functionalization of Phthalocyanines

Obed Rodriguez-Perez [a], Daniel Langerreiter [a], Sandra Kaabel [b], Eduardo Anaya-Plaza [c]

[a] *Department of Bioproducts and Biosystems. Aalto University. Kemistintie 1, 00016 AALTO, Finland*
[b] *Department of Chemistry and Materials Science. Aalto University. Kemistintie 1, 00016 AALTO, Finland*
[c] *Faculty of Medicine and Health Technology. Tampere University. Korkeakoulunkatu 3, Hervanta Campus, 33720 Tampere, Finland*

Phthalocyanines (Pcs) account for approximately 15–25% of the organic pigment market by volume, with an estimated annual production of several tens of kilotonnes in the EU and close to one hundred kilotonnes worldwide. However, their conventional synthesis and functionalization typically rely on solution-phase nucleophilic aromatic substitution (S_NAr) of phthalonitriles followed by cyclotetramerization, processes that require high-boiling solvents with recognized safety and environmental concerns, such as *N,N*-dimethylformamide (DMF) and 2-dimethylaminoethanol (DMAE). To address these limitations, we developed a solid-state strategy for the synthesis of functionalized phthalocyanines based on mechanochemistry and thermal aging, significantly reducing solvent consumption. Mechanochemical S_NAr under liquid-assisted grinding (LAG) was established as a robust and versatile platform for solvent-minimized functionalization of phthalonitriles. A broad substrate scope encompassing seven nucleophiles and nine electrophiles afforded mono-, di-, and tetrasubstituted phthalonitriles while enabling unique reactivity and selectivity. Furthermore, systematic screening of solid-state cyclotetramerization parameters clarified their roles in this reaction, using the conversion of tert-butyl phthalonitrile into tetra-tert-butyl phthalocyanine as a benchmark. Finally, the mechanochemical formation of phthalonitriles was seamlessly integrated with solid-state cyclotetramerization in both sequential and one-pot S_NAr–cyclotetramerization protocols, providing a versatile and more sustainable route to diverse phthalocyanine architectures.

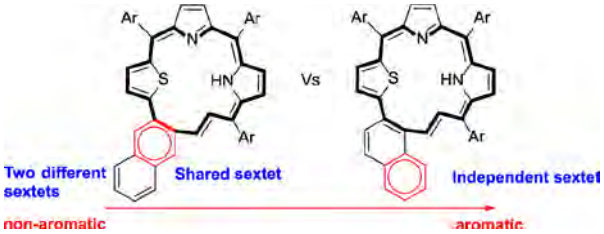
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Two Different Clar's Sextets: Clar's Rule Does Not Necessarily Contradict the Global Pathway of Conjugated Macrocycles

Tae-Ho Roh, Pradeep P. Desale, Min-Sung Ko, Dong-Gyu Cho*

Department of Chemistry and Chemical Engineering, Inha University



Two contradictory theories, Clar's sextet[1] and resonance theory[2], explain the stability of conjugated macrocycles using localized and delocalized models, respectively. To reconcile these theories and gain better insights, PAH-containing porphyrinoids were chosen as a representative class of conjugated macrocycles. Two types of Clar's sextets were identified and proposed for the first time based on their interaction with global conjugated pathways: (i) shared sextets that integrate with and perturb the global resonance pathway, and (ii) independent sextets that are separate from the pathway and potentially stabilize or do not perturb it. To test our hypothesis, we synthesized precise regioisomers with and without an independent sextet to exclude variables such as steric hindrance, different PAH characteristics, and other elements. This task is challenging due to the extensive synthetic efforts needed for regioisomeric PAH-containing porphyrinoids[3]. We focused on 2,3-vinylnaphthiporphyrin, which features shared sextets, because its o-regioisomers are readily accessible. Two distinct regioisomers (1,2-vinylnaphthiporphyrins) with an independent sextet were synthesized along with unexpected nonaromatic N-fused porphyrinoids. Our analysis shows that 1,2-vinylnaphthiporphyrins with an independent sextet are more aromatic than 2,3-vinylnaphthiporphyrin (nonaromatic). This sextet analysis was also applied to other reported and yet-to-be-synthesized PAH-containing porphyrinoids, and these results are consistent with our current study.

REFERENCES

1. Kumar, B.; Viboh, R. L.; Bonifacio, M. C.; Thompson, W. B.; Buttrick, J. C.; Westlake, B. C.; Kim, M.-S.; Zoellner, R. W.; Varganov, S. A.; Mörschel, P.; Teteruk, J.; Schmidt, M. U.; King, B. T. Septulene: The Heptagonal Homologue of Kekulene. *Angew. Chem., Int. Ed.* **2012**, *51*, 12795– 12800.
2. Herndon, W. C. Resonance energies of aromatic hydrocarbons. Quantitative test of resonance theory. *J. Am. Chem. Soc.* **1973**, *95*, 2404– 2406.
3. Hong, J.-H.; Aslam, A. S.; Ishida, M.; Mori, S.; Furuta, H.; Cho, D.-G. 2-(Naphthalen-1-yl)thiophene as a New Motif for Porphyrinoids: Meso-Fused Carbaporphyrin. *J. Am. Chem. Soc*. **2016**, *138*, 4992– 4995.

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Amphiphilic ABAC Phthalocyanine and its Potential Biomedical Applications

Rohlíčková, M.[a], Abraham, J. A.[b], Vávrová, P.[c], Konečná, K.[c], Kozlíková, M.[a], Zimčík, P.[b], Nováková, V.[b], Macháček, M.[a]

[a] *Department of Biochemical Sciences, Faculty of Pharmacy in Hradec Králové, Charles University, Czech Republic*
[b] *Department of Pharmaceutical Chemistry and Pharmaceutical Analysis, Faculty of Pharmacy in Hradec Králové, Charles University, Czech Republic*
[c] *Department of Biological and Medical Sciences, Faculty of Pharmacy in Hradec Králové, Charles University, Czech Republic*

In recent years, therapeutic approaches based on light activation become increasingly important in modern medicine. Photodynamic therapy (PDT) of malignant diseases is already clinically approved method. Nowadays because of the emergence and spread of multi-drug-resistant microorganisms, substantial attention has shifted toward photodynamic inactivation (PDI) of various microbial pathogens (also known as antimicrobial PDT), which is also clinically approved for selected localized applications, particularly in dentistry and nasal decolonization. PDI is an alternative treatment strategy that operates independently of antibiotic susceptibility. In this context, PDI represents a highly promising approach. Activated photosensitizers (PS) generate reactive oxygen species that effectively inactivate microorganisms through oxidative damage. This mechanism minimizes the risk of resistance development and thus makes PDI attractive for combating clinically relevant resistant pathogens [1]. Light-triggered strategies also include photochemical internalization (PCI), a technique designed to enhance intracellular drug delivery. PSs in PCI are specifically used for destabilization of endosomal membranes and thereby enabling the release of therapeutic macromolecules into the cytosol where they can reach their biological targets [2]. This project is focused on *in vitro* evaluation of effectiveness of novel highly asymmetric ABAC phthalocyanine PS in all abovementioned treatment modalities. Aside from excellent PDT activity against cancer cell lines (EC_{50} up to 89 nM), this PS also proved to be potentially suitable for PDI reaching 3-log reduction at 100 nM and MDC_{MRSA} at 1 μM. Although, the activity against *Klebsiella pneumoniae* was significantly lower. To better mimic physiological tissue architecture and evaluate toxicity against normal cells, a 3D dermal equivalent model consisting of fibroblasts embedded in extracellular matrix was employed. No detectable toxicity was found. Confocal microscopy of human skin detected only weak signal in *stratum corneum*. These findings demonstrate markedly improved safety in a physiologically relevant model and support the potential applicability for antimicrobial photodynamic treatment. Last but not least, as the compound is amphiphilic, it effectively facilitated PCI-mediated delivery of saporin into HeLa cells. Using the Chou-Talalay combination index method, we confirmed strongly synergistic effect.

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REFERENCES

1. Cieplik, F., Tabenski, L., Buchalla, W., & Maisch, T. (2014). Antimicrobial photodynamic therapy for inactivation of biofilms formed by oral key pathogens. *Frontiers in microbiology*, *5*, 405.
2. Weyergang, A., Selbo, P. K., Berstad, M. E., Bostad, M., & Berg, K. (2011). Photochemical internalization of tumor-targeted protein toxins. *Lasers in Surgery and Medicine, 43*(7), 721–733.

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Photophysical Characterizations for a Full Series of Novel Push-Pull Porphyrins Containing p-Aminophenyl and p-Carboxy/carbomethoxyphenyl Substituents.

Alexander B. Rudine[a], Brian D. DelFatti[a], Nicholas U. Day[a], and Carl C. Wamser[a]

[a]*Department of Chemistry, Portland State University, Portland, OR 97207-0751. USA*

Spectrophotometric titrations for a full series of *para*-amino/carbomethoxy-substituted tetraphenylporphyrins were carried out using methanesulfonic acid in DMSO to study the hyperporphyrin effect across different substitution patterns.[1] The series included zero, one, two (*cis* and *trans*), three, and four amino groups. With increasing numbers of p-aminophenyl groups, the relative basicity increased and the hyperporphyrin effect became more pronounced, as evidenced by a strong red band and a split Soret band. The *cis* diamino derivative was more readily protonated and showed a stronger hyperporphyrin effect compared to the *trans* isomer. For the monoamino derivative, an initial increase in the Soret band upon acid titration, along with well-defined isosbestic points, provided evidence for a monoprotonated porphyrin. The relative stability of this unusual intermediate is proposed to be due to charge delocalization of the first cation to the single amino group and destabilization of the second protonation by the electron-withdrawing carbomethoxy substituents. Upon saponification, the series of p-carboxy-substituted porphyrins and zinc porphyrins was studied as dyes for standard dye-sensitized solar cells (DSSCs).[2] The porphyrins with more amino groups generally showed higher efficiency, primarily due to higher photocurrents; open-circuit voltage and fill factors were comparable. The most efficient sensitizer was the *trans*-disubstituted zinc porphyrin, with an overall solar energy conversion efficiency of 5.66%, slightly higher than that of the triamino zinc porphyrin at 5.18%.

REFERENCES

1. Rudine AB, DelFatti BD, Wamser CC. *J. Org. Chem.* 2013; **78**: 6040-6049
2. Rudine AB, Day NU, Tian X, Lee C, James KE, Wamser CC. *J. Porphyrins Phthalocyanines* 2016; **20**: 1217-1223

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Synthesis, molecular structure and physicochemical properties of Si(IV) octapropylporphyrazine and etioporphyrin

Rychikhina E.D., Vyalkin D.A., Eroshin A.V., Zhabanov Y.A.

Ivanovo State University of Chemistry and Technology, RF-153000 Ivanovo, Russian Federation, e-mail: katyarychikhina@gmail.com

Porphyrazines belong to a broad class of π-conjugated tetrapyrrolic macrocycles, but have thus far received much less attention than their analogues bearing fused benzene rings (phthalocyanines) or aromatic heterocycles. Their physicochemical properties can be efficiently tuned through variation of both the nature of the central atom and the peripheral substituents. Among metal complexes of tetrapyrroles, silicon(IV) derivatives are of particular interest. Hexacoordinated silicon atom bears two axial coordination sites providing an additional route for structural tuning [1,2]. Despite extensive studies devoted to silicon(IV) phthalocyanines, silicon(IV) porphyrazines remain comparatively less explored, despite the fact that these compounds represent promising materials for applications in photomedicine and photovoltaics [1].

In this work, the Si(IV) octapropylporphyrazine and etioporphyrin-I was synthesized by complexation of corresponding metal free ligand with excess of trichlorosilane in the presence of triethylamine. After the reaction was complete, the axial chloride ligands were replaced by fluoride through treatment of crude product with hydrofluoric acid in dichloromethane leading to the formation of difluorosilicon(IV) octapropylporphyrazine $F_2SiPzPr_8$ and etioporppyrin-I $F_2SiEtioP$-I (Fig. 1).

The obtained compounds were characterized by UV-Vis, IR and ^1H NMR spectroscopy, their molecular structures were confirmed by single-crystal X-ray diffraction analysis. The effect of macrocyclic type on physicochemical properties is discussed. The electronic absorption spectra were simulated using quantum chemical calculations. In addition, luminescent and redox properties were investigated. For both complexes, a mass-spectrometric study of the sublimation process was carried out using the Knudsen effusion method. The sublimation enthalpy and entropy were found to be $\Delta_{subl}H$ = 191(4) kJ·mol^{-1} and $\Delta_{subl}S$ = 293(2) J·mol^{-1}K^{-1} for $F_2SiPzPr_8$ and $\Delta_{subl}H$ = 235(5) kJ·mol^{-1} and $\Delta_{subl}S$ = 392(3) J·mol^{-1}K^{-1} for $F_2SiEtioP$-I.

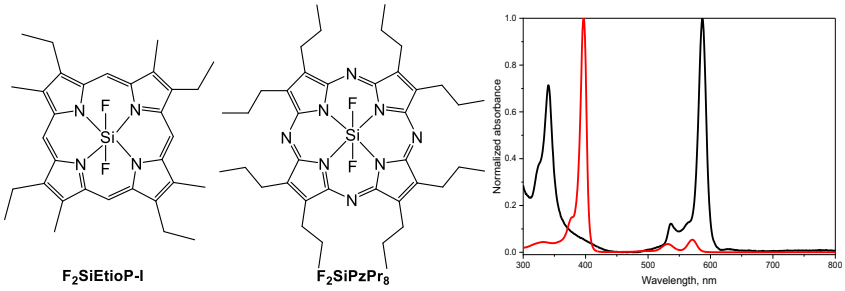


Figure 1. The structures of $F_2SiEtioP$-I and $F_2SiPzPr_8$, UV-Vis spectra of $F_2SiEtioP$-I (red) and $F_2SiPzPr_8$ (black) in CH_2Cl_2

This study was supported by RSF (grant No. 24-73-10107).

REFERENCES

1. K. Mitra, M.C.T. Hartman, Organic & Biomolecular Chemistry, **2021**, 19, 1168-1190.
2. J. E.Pia, et al. Coordination Chemistry Reviews, **2021**, 449, 214183.

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Si(IV) complexes of tetrapyrazinocorrolazine with camphor-annulated rings

Rychikhina E.D., Ivanova S.S., Stuzhin P.A.

Research Institute of Macroheterocycles, Ivanovo State University of Chemistry and Technology, RF-153000 Ivanovo, Russian Federation, e-mail: katyarychikhina@gmail.com

Silicon(IV) porphyrazines and corrolazines represent the tetrapyrrolic macrocycles that are structural *meso-aza*-analogues of porphyrins and corroles. Variation of axial ligand(s) at the silicon center in combination with peripheral functionalization of the macrocycle provides a convenient approach to tuning solubility, photophysical properties, singlet oxygen generation efficiency, etc. This structural flexibility makes these compounds attractive materials for development of photosensitizers, including systems intended for photodynamic therapy (PDT) [1].

In this work, Si(IV) complex of tetrapyrazinoporphyrazine with camphor-annulated rings ($(HO)_2$Si**Pz**) was obtained using both template tetramerization and complexation methods (Fig. 1) using modified procedures reported in [2,3]. Its treatment with chlorotripropylsilane in the presence of Mg in pyridine leads to contraction of porphyrazine macrocycle with formation the of corresponding corrolazine complex ((HO)Si**Cz**). Alternatively, (HO)Si**Cz** may be obtained with rather high yield (> 50 %) directly from metal free porphyrazine H_2Pz using $HSiCl_3$ and triethylamine.

The obtained compounds were characterized by UV-Vis, IR, ^{1}H NMR and CD spectroscopy. The effect of axial substituent (L=OH, F, Pr_3SiO, Ph_3SiO) and macrocycle contraction on the photophysical, photochemical, redox and acid-base properties of Si(IV) complexes was evaluated. Spectrophotometric titration data of LSi**Cz** with CF_3COOH reveal two consecutive protonation stages predominantly affecting *meso*-nitrogen atoms, whereas L_2Si**Pz** exhibited competitive protonation of *meso*- and pyrazine nitrogen atoms. Having a high ability to generate singlet oxygen (Φ_Δ=0.70), (Ph_3SiO)Si**Cz** can be considered as a promising photosensitizer for PDT.

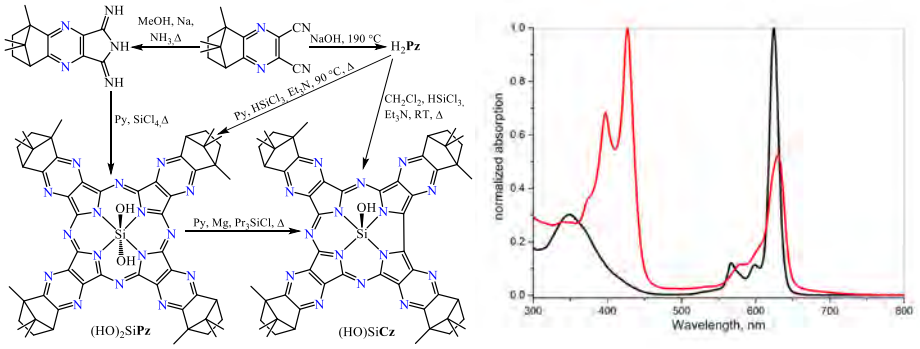


Figure 1. Scheme of synthesis of Si(IV) complexes and UV-vis spectra of (Ph3SiO)2Si**Pz** (black), (Ph3SiO)Si**Cz** (red) in CH2Cl2

This study was supported by the RSF (grant No. 25-23-01389).

REFERENCES

1. X.-F. Zhang, Coordination Chemistry Reviews, **2015**, 285, 52-64.
2. Jong min Park, Chang Young Jung, et al., Inorganic Chemistry Communications, **2015**, 62, 64–66.
3. M. Kolarova, P. Zimcik, et al., Journal of Porphyrins and Phthalocyanines, **2023**, 27, 444-451.

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BODIPY-Based Ligands for the Self-Assembly of Pd_nL_{2n} Coordination Cages.

A.Salazar[a], A. Mikherdov[b], G. Clever[b], G. de la Torre[a,c]

[a] *Department of Organic Chemistry, Universidad Autónoma de Madrid, Cantoblanco 28049, Madrid, Spain.*
[b] *Department of Chemistry and Chemical Biology, TU Dortmund University, Otto-Hahn-Str. 6, 44227 Dortmund, Germany.*
[c] *Institute for Advanced Research in Chemical Science (IAdChem), Cantoblanco 28049, Madrid, Spain.*

Coordination-driven self-assembly has generated a wide array of $\mathbf{Pd_nL_{2n}}$ coordination cages, enabling the predictable formation of well-defined nanoscale architectures with adaptable geometries and functions [1]. **BODIPY** derivatives are widely used as functional chromophores in supramolecular systems [2,3]; however, their potential as structural ligands for cage construction remains underexplored. The direct incorporation of BODIPY chromophores into defined cage architectures opens opportunities for controlled excited-state processes within confined supramolecular environments, offering perspectives toward triplet energy transfer systems and photocatalytic applications.

Here, we demonstrate that BODIPY-derived bis-monodentate ligands can act as structural elements in Pd_nL_{2n} cage assemblies. Variations in ligand design modulate nuclearity and topology, giving rise to discrete supramolecular architectures. The system further enables heteroleptic cage formation, expanding its structural scope and compositional flexibility (Figure 1).

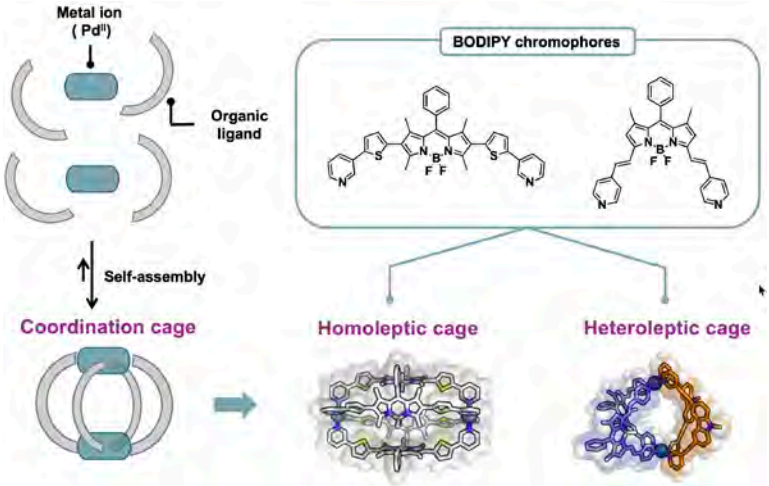


Figure1. Schematic representation of Pd^{2+}-driven self-assembly of BODIPY-based ligands into coordination cages, yielding either homoleptic or heteroleptic architectures depending on ligand composition.

REFERENCES

1. Neukirch, L.; Clever, G. H. *Chem. Sci*. 2025, **16**, 12242.
2. Durán-Sampedro, G.; Xue, E. Y.; Moreno-Simoni, M.; Paramio, C.; Torres, T.; Ng, D. K. P.; de la Torre, G. *J. Med. Chem.* 2023, **66**, 3448–3459.
3. Eng, L.; Huang, L.; Han, J.; Han, G. Acc. *Chem. Res*. 2022, **55**, 2604–2615.

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Magnetic Interaction in the Excited State of Triple-Decker Lanthanide Phthalocyanine Complexes

Anas Santria[a,b], **Yutaro Sakaguchi**[a], **Naoto Ishikawa**[a]

[a]*Department of Chemistry, Graduate School of Science, The University of Osaka*
[b]*Reseach Center for Molecular Chemistry, National Research and Innovation Agency*

Triple-decker lanthanide-phthalocyanine complexes have attracted attention due to their unique magnetic properties. While their ground-state behavior is well understood, their magnetism in the excited state has not been explored much. In this study, we investigated the excited-state magnetism of the PcLnPc*LnPc complex (where Pc* = 2,3,9,10,16,17,23,24-Octabutoxyphthalocyanine; Ln = Tb) using variable-temperature, variable-magnetic-field magnetic circular dichroism (VTVH-MCD) spectroscopy. The observed spectra exhibit anomalous magnetic response in the Q-band region, indicating an interaction between the orbital angular momentum generated by the ligand (**L**) and the total angular momentum generated by the 4f electronic system (**J**). The interaction was quantitatively analyzed by least-squares fitting of experimental A_1/D_0 ratios, using **J**-**L**, **J**-**J**, and |Lz| as parameters, where A_1 denotes the A-term intensity and D_0 the dipole strength.[1,2] The results indicate ferromagnetic-type **J**-**L** and **J**-**J** interactions for both at Q_H and Q_L. The **J**-**L** interaction in Q_L is stronger despite its smaller |Lz| value, compared to the interaction in the Q_H band, which implies increased localization of the orbital moments on the middle phthalocyanine. Ab initio multireference calculations support these findings and confirm the magnetic character of the excited states

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REFERENCES

1. K. Kizaki, H. Ozawa, T. Kobayashi, R. Matsuoka, Y. Sakaguchi, A. Fuyuhiro, T. Fukuda, N. Ishikawa, *Chem. Commun.* 2017, 53, 6168−6171.
2. T. Fukuda, H. Ozawa, Y. Sakaguchi, K. Kizaki, T. Kobayashi, A. Fuyuhiro, N. Ishikawa, *Chem. Eur. J.*, 2017, 23, 16357−16363.

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Monomer vs Dimer – Solvation and Aggregation Behaviour of two Octo-Carbazole Substituted Iron Phthalocyanines

Maximilian Schrodt[a], **Markus Enders**[a]

[a]*Institute of Inorganic Chemistry, Heidelberg University, Germany*

Ferrous iron in a square-planar coordination environment plays an important role in biology but also in so-called FeNC catalysts for the oxygen reduction reaction but the true nature of the active centres remains debatable. [1] We therefore explore FeN_4 model systems in which the iron centre is four-coordinate (i.e. no axial ligands present). Iron phthalocyanine and most of its derivatives are insoluble in non-coordinating solvents so that the axial positions are hardly accessible by reactants. We recently reported a well soluble, true four coordinate iron phthalocyanine and demonstrated that its paramagnetic ground state is triply degenerate due to strong spin-orbit coupling.[2, 3] Here, we present **1**H_2, an octo-di-*tert*-butyl-carbazole substituted phthalocyanine and its iron complex **1**Fe as well as their isomer **2**H_2 and **2**Fe which differ in the position of their *tert*-butyl groups. [4, 5]

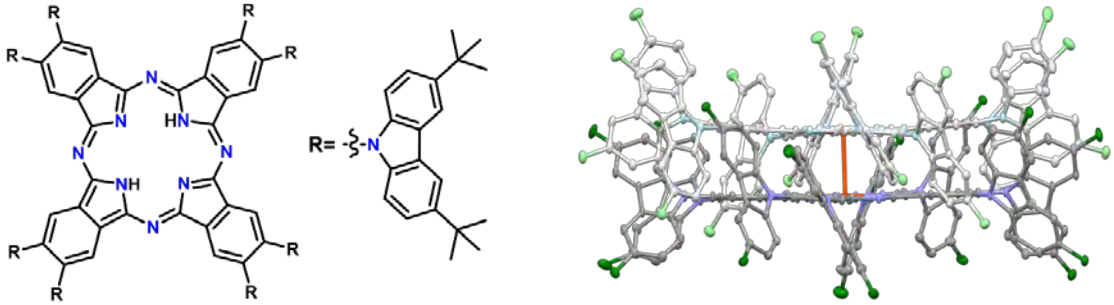


Figure: Structural formula of **1**H_2 (left) and the single-crystal XRD structure of the dimeric [**1**Fe] (with hydrogen atoms omitted and the 32 *tert*-butyl groups are represented by green points).

Unlike the monomeric **2**Fe, **1**Fe forms stable dimers with a weak iron-iron interaction in solution and in the solid state (Figure) showing no exchange signals of a monomer-dimer equilibrium in EXSY NMR, even at elevated temperatures (95 °C). The magnetic moment of **1**Fe (3.2 μ_B) is lower than that of to monomeric iron(II)-phthalocyanines like **2**Fe (3.7 μ_B). [2, 4]
We are now exploring the magneto-electronic structure of these compounds as well as their reactivity in redox processes and catalytic transformations.

REFERENCES

[1] K. Abdiaziz, L. Ni, D. Demirbas, H. Haak, E. Reijerse, P. Theis, W. Jiang, S. Chabbra, T. Lunkenbein, U. I. Kramm, A. Schnegg, *Journal of the American Chemical Society* **2026**.
[2] C. Iwanov, M. P. Hopp, D. Lorenz, J. Ballmann, M. Enders, *Chemistry – A European Journal* **2023**, *29*, e202302761.
[3] T. M. Diederich, T. Wehland, M. Schrodt, N. Kochetov, A. Schnegg, C. M. Jimenez-Muñoz, V. Krewald, L. Ni, N. S. Salas, U. I. Kramm, J. Ballmann, M. Enders, *Chemistry – A European Journal* **2025**, *31*, e202501474.
[4] M. Schrodt, J. Ballmann, M. Enders, *ChemRxiv* **2025**, *2025*.
[5] S. A. Majeed, B. Ghazal, D. E. Nevonen, P. C. Goff, D. A. Blank, V. N. Nemykin, S. Makhseed, *Inorganic Chemistry* **2017**, *56*, 11640-11653.

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Conformational flexibility of the nitrogenase-like reductase CfbC/D

Florian Schuhmacher[a], Lin Zhang[b], Alena Kussler[a], Oliver Einsle[c], Gunhild Layer[a]

[a]*Institute of Pharmaceutical Sciences, University of Freiburg, 79104 Freiburg, Germany.*
[b]*Faculty of Synthetic Biology, Shenzhen University of Advanced Technology, Shenzhen, 518107, China.*
[c]*Insitute of Biochemistry, University of Freiburg, 79104 Freiburg, Germany.*

Methanogenic archaea preserve energy anaerobically by the reduction of alternative electron acceptors, such as CO_2, acetate, methanol or methylamines to methane, a greenhouse gas known for its significant contribution to climate change. The terminal step in methanogenesis is catalyzed by methyl-coenzyme M reductase (MCR), which utilizes a unique Ni-containing porphinoid cofactor, called coenzyme F_{430} [1]. F_{430} is the most reduced tetrapyrrole found in nature and its biosynthesis from the precursor sirohydrochlorin is performed by the *coenzyme F_{430} biosynthesis* (*cfb*) gene products [2]. Among the F_{430} biosynthesis steps, the six-electron reduction of the macrocycle, catalyzed by the nitrogenase-like CfbC/D complex, became of particular interest over the past couple of years, not only due to the remarkable reaction, but also due to the high homology of CfbC/D to nitrogenase and nitrogenase-like enzyme systems, respectively [2-3]. Nitrogenase is the only biocatalyst that is able to reduce the chemically inert triple bond of nitrogen gas to form bioavailable ammonia under ambient conditions [4]. Similarly to nitrogenase, previously determined redox potentials of the CfbC (reductase) and CfbD (catalytic module) [4Fe:4S]-clusters indicate the need of a thermodynamically unfavourable "up-hill" electron transfer from the reductase onto the catalytic module [3]. In nitrogenase, this is possible due to structural rearrangements in the reductase module, NifH, upon ATP hydrolysis [4]. Interestingly, by combining structural data and *in silico* predictions, we obtained promising findings for major conformational changes in the catalytic subunit, CfbD, during the binding of the substrate, Ni-sirohydrochlorin-*a,c*-diamide (Ni-SHCD). This clearly distinguishes the CfbC/D complex from nitrogenase itself and other structurally characterized nitrogenase-like enzymes, such as dark operative protochlorophyllide reductase (DPOR) and methylthio-alkane reductase (MAR), which is mostly due to the simpler, tetrameric architecture of the CfbC/D complex. Based on these observations, we aim to study further on structural aspects of the CfbC/D complex, including a high-resolution structure of CfbD in the presence of Ni-SHCD, and the functional characterisation of the reaction mechanism by mutagenesis experiments. As the CfbC/D complex is proposed to be an ancient, archaeal precursor of nitrogenase, these findings and future investigations will shed a light not only on the biosynthesis of coenzyme F_{430}, but also on the evolutionary development of nitrogenase and its related enzyme systems.

REFERENCES

1. Chen H, Gan Q, Fan C. Methyl-Coenzyme M Reductase and Its Post-translational Modifications. Front Microbiol. 2020 Oct 9;11:578356.
2. Moore SJ, Sowa ST, Schuchardt C, Deery E, Lawrence AD, Ramos JV, Billig S, Birkemeyer C, Chivers PT, Howard MJ, Rigby SEJ, Layer G, Warren MJ. Elucidation of the biosynthesis of the methane catalyst coenzyme F_{430}. Nature. 2017 May 3;545(7652):116.
3. Vazquez Ramos J, et al. Characterization of the iron-sulfur clusters in the nitrogenase-like reductase CfbC/D required for coenzyme F_{430} biosynthesis. FEBS J. 2024 Jul;291(14):3233-3248.
4. Howard JB, Rees DC. Nitrogenase: a nucleotide-dependent molecular switch. Annu Rev Biochem. 1994;63:235-64.

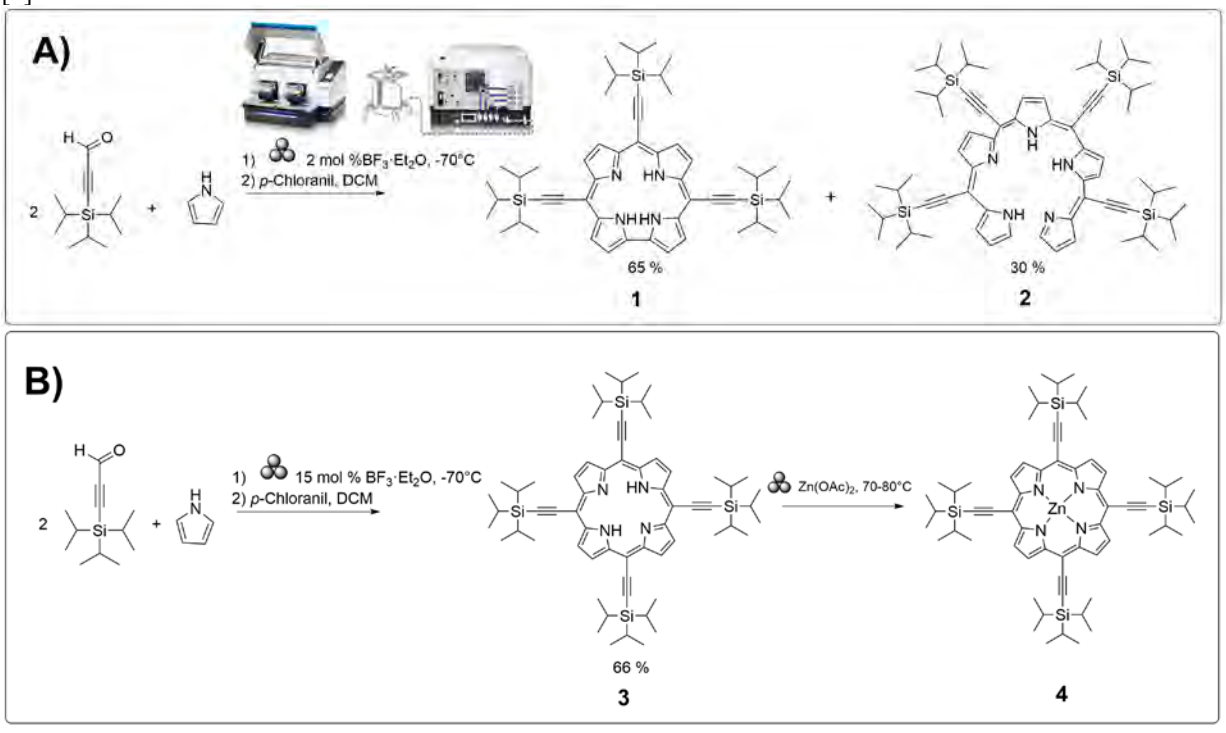
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Cro-Mechanochemical Synthesis of 5,10,15-Tris(isopropylsilylethynyl)-Corrole and 5,10,15,20-Tetrakis-((triisopropylsilyl)ethynyl)-Porphyrin

Wolfgang Schöfberger[a], **Sankit Vala, Houssein Awada, Simon Offenthaler, Adrian Dorniak**[a]

[a] *Johannes Kepler University Linz, Institute of Organic Chemistry, Altenberger Straße 69, 4040, Linz, Austria.*

We report a direct mechanochemical condensation of pyrrole with 3-(triisopropylsilyl)propiolaldehyde, followed by oxidation, to afford 5,10,15-tris((triisopropylsilyl)ethynyl)corrole **1** and 5,10,15,20-tetrakis-((triisopropylsilyl)-ethynyl)porphyrin **3** in up to 65% and 66% yield, respectively [1]. Using a temperature-controlled milling platform (Retsch MM 500 control with cryoPad), this method reduces total reaction time from ~12 h to 2 h and cuts reagent consumption by a factor of five compared to the standard Koszarna–Gryko protocol [2].



REFERENCES

1. Cryo-mechanochemical synthesis of free-base and metal A_3-corroles and A_4-porphyrins: A solvent-free approach, A. Dorniak and W. Schöfberger, Journal of Porphyrins and Phthalocyanines, 2025. https://doi.org/10.1142/S1088424625500208
2. B. Koszarna, D.T. Gryko, J. Org. Chem. 2006, 71, 3707-3717. https://doi.org/10.1021/jo060007k

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Cytochrome *c* as a target for metal-based anticancer drugs

Laura Cesati[a], Giulietta Smulevich[a,b], Maurizio Becucci[a,c], Lara Massai[a], Federico Sebastiani[a,b,c]

[b]*Department of Chemistry "U. Schiff", University of Florence, Via della Lastruccia 3, Sesto Fiorentino (FI), Italy*
[b]*INSTM, Research Unit of Florence, Via della Lastruccia 3, Sesto Fiorentino (FI), Italy*
[c]*The European Laboratory for Non-Linear Spectroscopy (LENS), Via N. Carrara 1, Sesto Fiorentino (FI), Italy*

Platinum-based drugs are widely used in chemotherapy, while gold-based drugs have recently emerged as a new class of anticancer compounds. Both families of metal-based drugs exert their cytotoxic effects by binding to proteins: gold compounds primarily target these biomolecules, whereas platinum-based drugs primarily target protein binding as a secondary mechanism [1, 2]. However, their molecular mechanism of action remains unclear.

Since these compounds are able to form stable adducts with cytochrome *c* [3], a mitochondrial protein involved in the initiation of cellular death [4], it is pivotal to explore the molecular interactions between metal-based drugs and this protein, as a possible therapeutic target.

Cyt *c* is one of the most studied heme proteins over the last 60 years, and it also serves as a model for fundamental folding and unfolding processes [5]. During unfolding, cyt *c* can adopt a variety of non-native states characterized by conformational rearrangements [6], which, interestingly, are also observed upon binding to cardiolipin (CL). CL is a phospholipid of the inner mitochondrial membrane, which mediates the anchoring of cyt *c* to the membrane itself and participates in the steps preceding apoptosis [7].

We have explored the interactions of selected metal compounds, either with promising anticancer activity or with well-established clinical use, with cytochrome *c* by the combination of mass spectrometry (for adduct formation and stoichiometry), circular dichroism (for the secondary structure alteration), UV-vis electronic absorption and resonant Raman (for electronic and vibrational characterization of the active site and ligand binding to heme cofactor) spectroscopies. In particular, the aim is to understand whether and how these interactions induce conformational changes of cytochrome c, possibly related to its proapoptotic function.

REFERENCES

1. J. Bogojeski, B. Petrović and Z.D. Bugarčić – Chapter 16 in "Chronic Lymphocytic Leukemia" - Ed. by P. Oppezzo (2012), Intech Open Publishing
2. Z.D. Bugarčić, J. Bogojeski, B. Petrović, S. Hochreuther,, R. van Eldik - Dalton Trans. (2012) 41, 12329.
3. C. Gabbiani, L. Massai, F. Scaletti, E. Michelucci, L. Maiore, M.A. Cinellu, L. Messori - J. Biol. Inorg. Chem. (2012) 17, 1293-1302.
4. Y-L.P. Ow, D.R. Green, Z.Hao, T.W. Mak - Nature Reviews Molecular Cell Biology (2008) 9, 532–542.
5. S.R. Yeh, D.L. Rousseau, Nature Structural Biology (1998) 5, 222-228.
6. L. Milazzo, L. Tognaccini, B.D. Howes, G. Smulevich – J. Raman Spectrosc. (2018) 49, 1041-1055.
7. D. Mohammadyani, N. Yanamala, A.K. Samhan-Arias, A.A. Kapralov, G. Stepanov, N. Nuar, J. Planas-Iglesias, N. Sanghera, V.E. Kagan, J. Klein-Seetharaman – Biochim. Biophys. Acta Biomembr. (2018) 860, 1057-1068.

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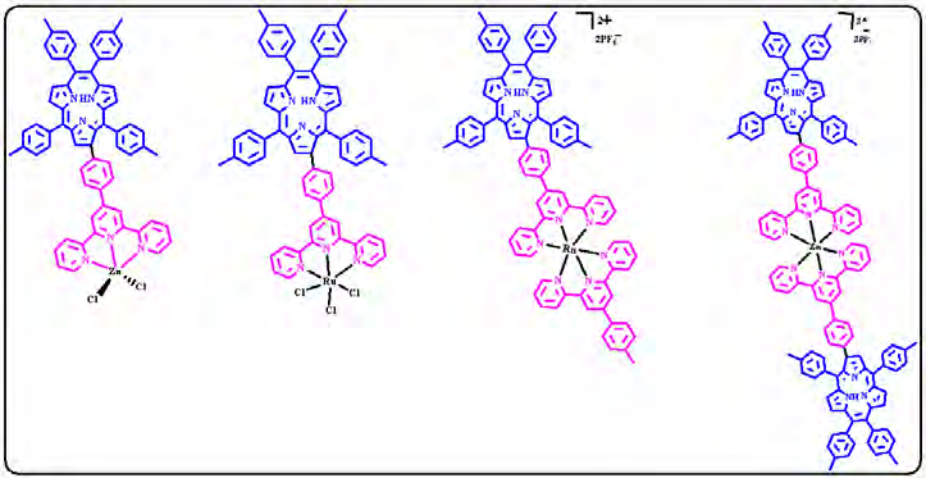


Synthesis of β-Terpyridinyl Triphyrin(2.1.1) and its coordination chemistry

Gayathri Sekar[a] and Mangalampalli Ravikanth*[a]

[a]*Department of Chemistry, Indian Institute of Technology, Bombay 400076, India.*
E-mail: gayuchem96@gmail.com

Meso-tetraaryltriphyrin(2.1.1)s are contracted aromatic14π-electron porphyrinoids composed of three pyrrole rings linked by four meso carbons[1, 2]. Unlike conventional 18π-electron porphyrins, these systems possess a smaller cavity, one less pyrrole unit, and only one ionizable proton. Their coordination chemistry remains less explored due to the restricted inner cavity and strong intramolecular hydrogen bonding, which hinder metallation. Although efficient synthetic methods were reported nearly a decade ago, the literature on meso-tetraaryltriphyrin(2.1.1)s remains limited. In my poster, I will present the synthesis and properties of selected covalently linked β-terpyridinyl triphyrin(2.1.1) ligands and their coordination complexes [3-6].



Keywords: Terpyridine; Triphyrin(2.1.1), Coordination complexes

REFERENCES

1. S. Shimizu, Chem. Rev., 2017, **117**, 2730–2784.
2. D. Kuzuhara, H. Yamada, Z. L. Xue, T. Okujima, S. Mori, Z. Shen and H. Uno, Chem. Commun., 2011, **47**, 722–724.
3. G. Kaur and M. Ravikanth, Adv. Heterocycl. Chem., 2023, **140**, 171–231.
4. D. Kuzuhara, Z. Xue and S. Mori, Chem. Commun., 2013, **49** 8955–8957.
5. K. N. Panda, R. Sengupta, A. Kumar and M. Ravikanth, J. Org. Chem., 2021, **86**, 3778–3784.
6. A. Sharma and M. Ravikanth, Dalton Trans., 2025, **54**, 6935–6945.

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Highly-Conjugated Porphyrin Polymer Films via Oxidative Chemical Vapor Deposition for the Oxygen Reduction Reaction

Emut Sukma Sejati[a], Amr Nada[a], Nicolas D. Boscher[a], Diego Martinez-Martinez[a], Robin J. White[a]

[a]*Luxembourg Institute of Science and Technology (LIST), 28, Avenue des Hauts-Fourneaux, L-4362 Esch-sur-Alzette, Luxembourg*

The potential of porphyrins, especially those with metal centres (e.g. Co, Ni, and Fe), is well known for catalysing oxygen reduction reaction (ORR) [1]. Extended conjugated porphyrin assemblies have been reported to exhibit superior catalytic activity than their monomeric counterparts. However, their limited solubility restricts solution-based processing and inhibits deposition of extended conjugated structures onto solid substrates. To address this challenge, oxidative chemical vapor deposition (oCVD) offers a route to the on-substrate formation of highly conjugated fused porphyrin polymers [2]. $FeCl_3$ has been reported as the most efficient oxidant to grow multiply-fused porphyrin chains under relatively mild conditions [3,4]. However, residual $FeCl_3$ and associated by-products generate uncontrolled aggregates within the resulting thin films [2]. To mitigate this, post-deposition washing using ethanol and dilute acid was employed following the deposition of Co, Ni, and Fe-based fused porphyrin polymers via oCVD (e.g. on FTO glass substrates). Ethanol washing was found not to remove residual $FeCl_3$, as evidenced by scanning electron microscopy and electron dispersed X-ray Spectroscopy (SEM-EDX). In contrast, acid washing removed residues as confirmed by SEM-EDX and X-ray Photon Spectroscopy (XPS). High resolution mass-spectroscopy revealed no or only minor demetallation of acid washed-fused porphyrin polymers depending on metal centre, whilst the conjugated polymeric backbone in all cases remained intact. The retention of long conjugation was confirmed by higher absorption near infrared region (NIR), with UV/Vis/NIR spectra being identical for both washed and unwashed samples. XPS also confirmed retention of identical chemical environment(s) (e.g. for metal centres) for oCVD deposited material and washed counterparts. The deposited porphyrin-based materials were electrochemically characterised under ORR conditions. Interestingly, residue washing significantly enhanced ORR catalytic performance, particularly for fused Ni-porphyrin polymer in alkaline electrolyte, as evidenced by cyclic voltammetry, electrochemical impedance spectroscopy, and chronopotentiometry. Finally, the fused porphyrin polymers are evaluated in lab-scale fuel cell system.

REFERENCES

1. Y. Cao, Y. Mou, J. Zhang, R. Zhang, and Z. Liang, Materials Today Catalysis, vol. 4, p. 100044, 2024, doi: https://doi.org/10.1016/j.mtcata.2024.100044.
2. D. Cardenas-Morcoso, E. Vey, M. Heiderscheid, G. Frache, and N. D. Boscher, J. Mater. Chem. C, vol. 10, no. 6, pp. 2194–2204, 2022, doi: 10.1039/D1TC05452J.
3. D. Cardenas-Morcoso, D. Bansal, M. Heiderscheid, J.-N. Audinot, J. Guillot, and N. D. Boscher, ACS Catal, vol. 13, no. 22, pp. 15182–15193, Nov. 2023, doi: 10.1021/acscatal.3c02940.
4. K. Chowdhury, S. K. Behura, M. Rahimi, and M. Heydari Gharahcheshmeh, ACS Appl Energy Mater, vol. 7, no. 3, pp. 1068–1079, Feb. 2024, doi: 10.1021/acsaem.3c02589.

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Synthesis of *β*-Substituted *Meso*-Tetraaryl Triphyrin(2.1.1)s and Covalently Linked Triphyrin(2.1.1)-Porphyrin Dyads

Akrti Sharma[a], **M. Ravikanth**[a]

[a]*Department of Chemistry, Indian Institute of Technology, Powai, Mumbai 400076, India*
E-mail: ravikanth@chem.iitb.ac.in

Triphyrin(2.1.1)s are contracted congeners of porphyrins containing three pyrrole rings connected *via* four *meso* carbons in 14π electron conjugation [1]. We developed conditions for regioselective bromination of triphyrin(2.1.1). Notably, slight adjustments in the reaction conditions resulted in the formation of unsymmetrical tetrabromo triphyrin, which was then used to synthesize sterically crowded octaarylated triphyrins [2] (**I**). Further, sterically crowded decaaryl triphyrins [3] (**II**) were synthesized by coupling *β*-hexabromo triphyrin(2.1.1) with various arylboronic acids. A series of *β*-arylated triphyrin(2.1.1)s (**III**) with varying number of *p*-fluorophenyl groups from one to six were synthesized, and explored their structure, spectral and redox properties [4]. Then, a series of antiaromatic P^{V}=O complexes of triphyrin (**IV**) and its *β*-substituted derivatives were synthesized [5]. Next, the first examples of covalently linked, *β*-*meso*-phenyl ethyne bridged hybrid dyads (**V**) containing 14π triphyrin(2.1.1)/metallotriphyrin and 18π porphyrin/metalloporphyrin subunits were synthesized [6]. Lastly, we attempted to synthesize N-methyl *meso*-tetraaryltriphyrin(2.1.1)s (**VI**) under methylation reaction conditions and the presence of the methyl group on inner core nitrogen of triphyrin(2.1.1) induces significant distortion in the 14π macrocycle. The synthesis, spectral, electrochemical, and theoretical studies of all these compounds will be discussed in the poster presentation.



REFERENCES

1. Panda, K. N.; Thorat, K. G.; Ravikanth, M. *J. Org. Chem.* **2018**, *83*, 12945-12950.
2. Sharma, A.; Kaur, G.; Ravikanth, M. *Org. Biomol. Chem.* **2024**, *22*, 838-849.
3. Sharma, A.; Alka, A.; Ravikanth, M. *Chem. Asian J.* **2024**, *19*, e202400799.
4. Sharma, A.; Ravikanth, M. *Tetrahedron* **2024**, *168*, 134349.
5. Sharma, A.; Ravikanth, M. *Dalton Trans.* **2025**, *54*, 6935-6945.
6. Sharma, A.; Alka, A.; Ravikanth, M. *Chem. Asian J.* **2025**. (In-press).

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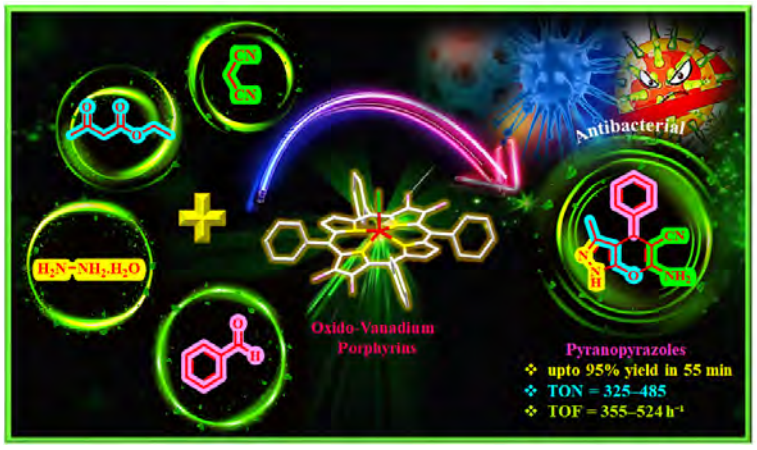


β-Functionalized Oxido-Vanadium Porphyrins for Multicomponent Synthesis of Bioactive Pyranopyrazoles

Shivani, and Muniappan Sankar*

Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 24667, India

Multicomponent reactions (MCRs) offer a sustainable and atom-economical approach to heterocyclic synthesis.[1] In this study, three *β*-substituted oxido-vanadium porphyrins, *viz*. VOTPP, VOTPPBr$_4$, and VOTPPMe$_4$ were evaluated as catalysts for the four-component synthesis of bioactive pyranopyrazoles. The catalytic performance was found to be strongly dependent on *β*-substitution. Among the three complexes, VOTPPBr$_4$ exhibited the highest efficiency, affording up to 95% yield with shorter reaction time, as well as higher turnover numbers (TON: 325–485) and turnover frequencies (TOF: 355–524 h^{-1}). In contrast, VOTPP showed moderate activity, while VOTPPMe$_4$ displayed reduced efficiency, consistent with their respective reduction potentials and redox behavior. Importantly, all catalysts retained structural integrity and activity over five successive cycles, highlighting their recyclability.[1e] Single-crystal X-ray diffraction analysis of VOTPPMe$_4$ confirmed a distorted porphyrin macrocycle, consistent with theoretical predictions. Density functional theory calculations revealed that bromine substituents in VOTPPBr$_4$ stabilize the LUMO, enhancing Lewis acidity and carbonyl activation for efficient pyranopyrazole formation, whereas methyl groups destabilize the LUMO and reduce activity. Thus, catalytic behavior is governed by the interplay of macrocyclic distortion and LUMO stabilization, highlighting *β*-substitution as a key handle for tuning vanadium porphyrin catalysis.[1e]



REFERENCES

1. (a) Cioc RC, Ruijter E, Orru, *Green Chem.* **2014**, *16*, 2958-2975. (b) M. R. Maurya, S.K. Maurya, N. Kumar, F. Avecilla, *J Org Chem*. **2024**, *89*, 12143-12158. (c) S.K. Yadav, A. Patter, M. Sankar, *Inorg Chem.* **2024**, *63*, 11102–11112. (d) Yadav SK, Kumar N, Sankar M., *Inorg Chem.* **2025**, 64, 11907-11924. (e) S. Rathi, and M. Sankar, *Manuscript Submitted for Publication.*

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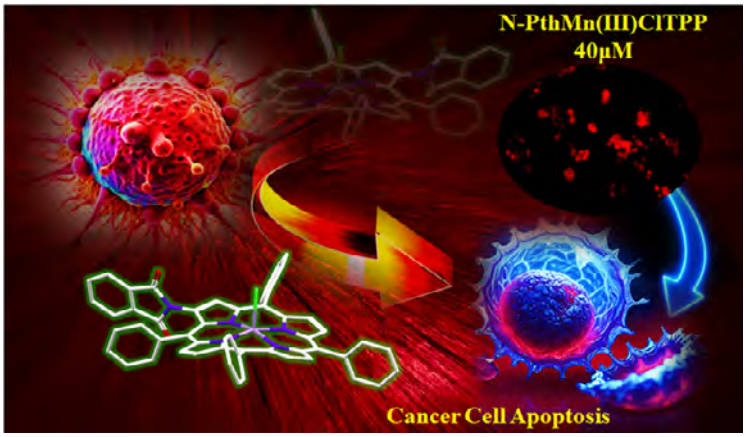
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β-Substituted Phthalimide Porphyrins as Redox-Active Anticancer Agents Against HeLa Cells

Shivani, and Muniappan Sankar*

Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247667, India

Porphyrins are versatile tetrapyrrolic scaffolds whose structural and electronic tunability makes them attractive candidates for anticancer applications.[1] Herein, a newly developed *β*-substituted free-base phthalimide porphyrin and its manganese analogue were synthesized and structurally characterised to assess their anticancer properties. *β*-Pyrrolic functionalization was employed to tune the electronic properties of the porphyrin core, while coordination of manganese and attachment of a phthalimide fragment were intended to influence redox characteristics and intermolecular interactions relevant to biological activity.[1] The antiproliferative effects of both porphyrins were examined in human cervical carcinoma (HeLa) cells. *In vitro* studies revealed that the manganese phthalimide porphyrin exhibited higher cytotoxicity, reducing cell viability by over 50% at 40 μM, while the free-base phthalimide porphyrin required 100 μM to achieve similar effects, demonstrating a clear dose-dependent response in MTT assays.[1d] Fluorescence-based AO/EtBr staining demonstrated apoptosis as the dominant mode of cell death, and enhanced intracellular reactive oxygen species (ROS) generation was observed using DCFDA probes. The presence of the phthalimide moiety appears to support cellular association and oxidative stress induction, thereby amplifying ROS-mediated apoptotic pathways. These findings suggest that *β*-substituted manganese phthalimide porphyrins represent a promising structural motif for the development of porphyrin-based anticancer agents.[1d]



REFERENCES

1. (a) M. Ethirajan, Y. Chen, P. Joshi, R.K. Pandey, *Chem. Soc. Rev.* **2010**, *40*, 340–362. (b) A.D. Hendsbee, S.M. McAfee, J.P. Sun, T.M. McCormick, I.G. Hill, G.C. Welch, *J. Mater. Chem. C* **2015**, *3*, 8904–8915. (c) C. D'Alfonso, M. Bietti, G.A. Dilabio, O. Lanzalunga, *J. Org. Chem.* **2013**, *78*, 1026–1037 (d) S. Rathi, and M. Sankar, *Manuscript Submitted for Publication*.

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Stepwise Nitrate → Dinitrogen Transformation Mediated by a Series of Synthetic Heme/Cobalt and Heme/Copper Assemblies: Modeling Denitrification with Cytochrome c Oxidase Mimics

Shubham[a], **Pritam Mondal**[a]

[a]*Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Punjab 140306, India.*

Nitrogen oxides (NO_x) are key players in numerous physiological, pathological, ecological, and environmental processes, undergoing reductive transformations from nitrate (NO_3^-) to diatomic nitrogen (N_2) via intermediates such as nitrite (NO_2^-), nitric oxide (NO) and nitrous oxide (N_2O).[1] While nature employs various enzymatic systems for these transformations,[2] the mechanistic details remain largely unclear, and synthetic models to replicate these processes are scarce. In this work, we introduce partially reduced heme/copper and heme/cobalt complexes that effectively reduce NO_3^- to NO_2^- and ultimately produce NO in a stepwise manner. We demonstrate the reductive coupling of NO to N_2O using Lewis acid or heme/copper assemblies, marking the successful conversion of N_2O to N_2 for the first time with reduced heme/non-heme assemblies. Additionally, we explore the oxidation of NO to NO_2^- and NO_2 to NO_3^- using μ-oxo heme-Fe^{III}–O–M^{II} (M: Co/Cu) complexes. Our findings, characterized through techniques such as UV-Visible spectroscopy, ^{2}H-NMR, EPR, FT-IR spectroscopy, mass spectrometry, and ^{15}N-labeling experiments, provide valuable insights into the role of heterobinuclear heme/non-heme centers in NO_x transformations and clarify the mechanistic pathways involved in biological NO_x-converting enzymes.[3]

REFERENCES

1. M. J. Pennino, J. E. Compton, S. G. Leibowitz, *Environ. Sci. Technol*., 2017, **51**, 13450–13460.
2. N. Lehnert, B. W. Musselman, L. C. Seefeldt, *Chem. Soc. Rev*., 2021, **50**, 3640−3646.
3. Shubham, P. Mondal, *JACS Au*. 2025, **5**, 4773−4787.

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Exploring Hydrogen Atom Abstraction Thermodynamics of a Synthetic (Heme)Fe^{III}–OH Complex: Understanding the Mechanistic intricacies of the final step of Heme-copper Oxidases

Shubham[a], Pritam Mondal[a]

[a]*Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Punjab 140306, India. E-mail: pritam@iisermohali.ac.in*

Abstract Start. Heme-copper oxidases (HCOs) are terminal enzymes on the mitochondrial or bacterial respiratory electron transport chain, which utilize a unique heterobinuclear active site (Heme-$Fe^{II}\cdots Cu^{I}$) to catalyze the $4H^{+}/4e^{-}$ reduction of dioxygen to water.[1] The final step of the proposed mechanistic pathway involves a (heme)Fe^{III}-OH intermediate that is reduced (taking up an electron and a proton) to form the reduced enzyme state, along with one water molecule.[2] Nonetheless, the exact mechanistic details of these terminal oxidases remain poorly understood. Although computational studies of such bimetallic active sites in the heme-copper oxidases have been presented [3], definitive experimental evidence for those proposed pathways is lacking. In this work, we present a detailed investigation into the hydrogen atom abstraction (HAA) reactivity of a synthetic (heme)-Fe^{III}-hydroxo species using a weak O–H bond substrate, TEMPO–H, resulting in the corresponding heme Fe^{II} adduct, and one equivalent of water, paralleling similar observations in the enzyme. Such HAA reactivity has been substantiated through rigorous thermodynamic and kinetic investigations, which reveal the bond-dissociation free energy of the complex. These experimental findings are further corroborated by theoretical investigations, and both are in strong agreement with the observed reactivity pattern. Such crucial findings in understanding the final step of the mechanistic pathways of heme-copper oxidases will be discussed in detail.

REFERENCES

1. Adam, S. M.; Wijeratne, G. B.; Rogler, P. J.; Diaz, D. E.; Quist, D. A.; Liu, J. J.; Karlin, K. D. *Chem. Rev.* **2018**, *118*, 10840.
2. Blomberg, M. R. A. A.; Siegbahn, P. E. M. *Biochim. Biophys. Acta, Bioenerg*. **2015**, *1847*, 1173−1180.
3. Bloch, D.; Belevich, I.; Jasaitis, A.; Ribacka, C.; Puustinen, A.; Verkhovsky, M. I.; Wikström, *M. Proc. Natl. Acad. Sci. U. S. A.* **2004**, *101*, 529−533.

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Synthetic Strategies Towards Phthalocyanine–Lipoic Acid Conjugates

Dilara Sipahioğlu[a] **and Fabienne Dumoulin**[a,b]

[a] *Acıbadem Mehmet Ali Aydınlar University, Graduate School of Natural and Applied Sciences, Department of Biomedical Engineering, 34752, Istanbul, Türkiye*
[b] *Acıbadem Mehmet Ali Aydınlar University, Faculty of Engineering and Natural Sciences, Department of Biomedical Engineering, 34752, Istanbul, Türkiye*

Lipoic acid is a naturally occurring organosulfur compound with a five-membered cyclic disulfide ring and a terminal carboxylic acid group. These features give it unique redox activity and broad chemical reactivity. Its reversible disulfide–dithiol transformation allows strong Au–S bond formation with gold surfaces, supporting its use in gold nanoparticle stabilization, surface functionalization, self-assembled monolayer formation, and biosensing interfaces. In addition to gold-based systems, lipoic acid is used in various nanostructured materials and redox-responsive platforms due to its metal-binding affinity, amphiphilic properties, and ability to form covalent conjugates [1-4]. It has already axially substituted a subphthalocyanine for this kind of purpose [5].

Strategies for preparing phthalocyanine-lipoic acid conjugates with lipoic acid on the periphery of the macrocycle will be discussed.

REFERENCES

1. Doi, A.; Sahu, M.; Sharma, P.; Ganguly, M. Role of Lipoic Acid and Gold Nanomaterials and Nanoclusters for Biomedical and Environmental Applications. *Mater. Res. Bull.* **2026**, *193*, 113712.
2. Eberle, C. S.; Viana, A. S.; Montforts, F.-P.; Abrantes, L. M. Synthesis and Self-Assembly of a Novel Cobalt(II) Porphyrin Lipoic Acid Derivative on Gold. *J. Porphyr. Phthalocyanines* **2010**, *14* (01), 101–107.
3. Martin-Trasanco, R.; Cao, R.; Montforts, F.-P. Self-Assembly of a Ru(II)-Deuteroporphyrin Lipoic Acid Derivative on Au(111) Surfaces. *J. Porphyr. Phthalocyanines* **2015**, *19* (09), 1014–1020.
4. Blas-Ferrando, V. M.; Ortiz, J.; Fernández-Lázaro, F.; Sastre-Santos, Á. Synthesis and Characterization of a Sulfur-Containing Phthalocyanine-Gold Nanoparticle Hybrid. *J. Porphyr. Phthalocyanines* **2014**, *19* (01n03), 335–343.
5. González-Rodríguez, D.; Martínez-Díaz, M. V.; Abel, J.; Perl, A.; Huskens, J.; Echegoyen, L.; Torres, T. Self-Assembled Monolayers of Subphthalocyanines on Gold Substrates. *Org. Lett.* **2010**, *12* (13), 2970–2973.

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Zinc Phthalocyanine and Gadolinium Co-Loaded Liposomes as a Platform for Magnetic Resonance Imaging and Photodynamic Treatment

Lukasz Sobotta[a], Paulina Skupin-Mrugalska[a], Daniel Ziental[a]

[a]*Department of Inorganic and Analytical Chemistry, Poznan University of Medical Sciences, Rokietnicka 3, 60-808 Poznan, Poland*

Liposomes are widely recognized as versatile drug delivery systems due to their ability to encapsulate both hydrophilic and lipophilic compounds. Their composition can be easily modified by incorporating different phospholipids and functional additives, enabling the development of multifunctional nanoplatforms that combine diagnostic and therapeutic capabilities. In this study, gadolinium-incorporated liposomes (GdLip) were developed for the simultaneous delivery of a magnetic resonance imaging (MRI) contrast agent and a photosensitizer intended for photodynamic therapy (PDT).

GdLip were prepared using the conventional thin-film hydration method. The singlet oxygen quantum yield of zinc phthalocyanine incorporated into GdLip was evaluated to determine whether the presence of gadolinium ions affects photodynamic activity. The results demonstrated that singlet oxygen generation remained unchanged in the presence of gadolinium. Longitudinal (r1) and transverse (r2) relaxivity parameters were determined at different proton resonance frequencies. The obtained values indicate that GdLip exhibit promising contrast-enhancing properties, influencing both T1 and T2 relaxation times. T2-weighted MRI images confirmed a significant contrast enhancement compared to blank liposomes.

In vitro studies were performed to assess cytotoxicity under dark conditions and following light irradiation. GdLip showed no significant toxicity toward HeLa cancer cells and normal human fibroblasts in the absence of light. In contrast, light exposure resulted in a reduction of cell viability by more than 90%, confirming effective photodynamic activity.

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Molecular materials for carbon capture and storage: On-surface characterisation of self-assembly and gas adsorption properties of metal phthalocyanines and porphyrins.

Joseph Straw[1], Matthew Edmondson[1], Michael Clarke[2], Liv Warwick[1], Ailish Gray[1], Amelia Thompson[1,3], Fulden Eratam[3], David A. Duncan[2,3], Alex Saywell[1]

[1]*School of Physics and Astronomy, University of Nottingham, UK*
[2]*School of Chemistry, University of Nottingham, UK*
[3]*Diamond Light Source, Oxfordshire, UK*

The successful capture and storage of pollutant gases, including the carbon and nitrogen containing compounds produced by industrial processes (e.g. CO_2 and NO_x), is of significant environmental importance. The synthesis and characterisation of materials which enable gas sequestration is therefore of interest and offers a promising route to limiting the effects of climate change. Molecular based materials containing functional moieties which can ligate, and trap gases are of particular utility in this regard and may provide a way of selectively and efficiently removing pollutants. Here we study molecular arrays of cobalt phthalocyanine (CoPc) and cobalt tetraphenylporphyrin (CoTPP) on Ag(111) and study oxygen ligation at the metal centres of these molecules. Metal functionalised porphyrins and phthalocyanines (Pcs) have been extensively studied in ultra-high vacuum (UHV) conditions [1], and the ligation (and reaction) of gases at the metal centre has been observed [2-4]. Interestingly, conformational flexibility is known to be strongly correlated with entropic factors which promote enhanced reaction rates within biological systems [5]. We therefore investigate a biomimetic approach to enhance reactivity by switching from a rigid Pc system to a flexible TPP. We employ UHV scanning tunnelling microscopy (UHV-STM), X-ray photoelectron spectroscopy (XPS) and X-ray standing wave (XSW) to characterise the morphology, chemistry and adsorption height of the on-surface self-assembled structures (in a similar approach to our previous work [6-7]) and investigate the chemical and structural changes which both molecules undergo following the exposure of the respective systems to oxygen.

REFERENCES

1. J. M. Gottfried, *et al. Surf. Sci. Rep*. **70**, 259 (2015)
2. E. Vesselli, *et al. J. Phys. Mater*. **3**, 022002 (2020)
3. D. Nguyen, *et al. J. Am. Chem. Soc*. **140**, 18 (2018)
4. J. Qiao, *et al. Chem. Soc. Rev*. **43**, 2 (2014)
5. J. Åqvist, *et al. Acc. Chem. Res*. **50**, 2 (2017)
6. C.J. Judd, *et al. Commun Chem.* **3**, 166 (2020)
7. E.S. Frampton, *et al. Inorganica Chim. Acta.* **558**, 121718 (2023)

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Electrospray deposition and on-surface characterisation of cyclic-porphyrin polymers

Joseph Straw[1], Matthew Edmondson[1], Michael Clarke[1], James N. O'Shea[1], Harry L. Anderson[2], Alex Saywell[1]

[1]School of Physics and Astronomy, University of Nottingham, UK
[2]Department of Chemistry, Oxford University, UK

Synthetic chemistry provides a way to 'build' complex functional molecules by precisely arranging atomic species and chemical groups. However, confirming successful synthesis of large/complex target molecules (for example, by definitively determining morphology and structure) can be non-trivial. Over the last few years developments in electrospray deposition (ESD) have allowed a range of thermally labile/non-volatile molecules to be transferred from solution to substrates held under ultra-high vacuum (UHV) conditions for characterisation by scanning probe microscopy (SPM) techniques. [1-3] This approach allows the sub-molecular level spatial characterisation offered by SPM to be combined with the chemical specificity of photoelectron spectroscopies and provides details complementary to the characterisation techniques frequently used to analyse the products of organic synthesis (e.g. UV-VIS spectroscopy and NMR).

Here we present details of our studies of cyclic porphyrin polymers ('nanorings') characterised by UHV-SPM. The nanorings have been observed to display a range of interesting optical [4] and electronic properties [5], including global (anti) aromatic ring currents for nanorings with even (odd) numbers of porphyrins. [6] Specifically, we focus on the geometry, flexibility and chemical characterisation of electrospray-deposited cyclic polymers using UHV-SPM and X-ray photoelectron spectroscopy (XPS).

REFERENCES

1. A. Saywell, *et al. Nat. Commun.* **1**, 75 (2010)
2. S. Rauschenbach, *et al. ACS Nano.* **3**, 10 (2009)
3. S. Moro, *et al. ACS Nano.* **16**, 12 (2022)
4. H. Gotfredsen, *et al. Nat. Chem*. **14** (2022)
5. C.J. Judd, *et al. Phys Rev Lett.* **125** (2020)
6. A. Rodríguez-Rubio, *et al. Sci.* **390**, 6770 (2025)

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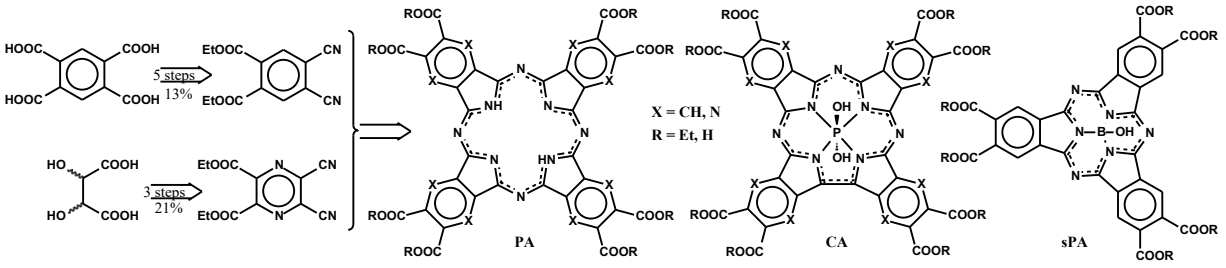


Contracted and azaanalogues of peripherally carboxylated phthalocyanine

Ekaterina S. Gnedina, Dmitriy A. Lazovskiy, Ivan A. Nikitin and Pavel A. Stuzhin

Research Institute of Macroheterocycles, Ivanovo State University of Chemistry and Technology, RF-153000, Ivanovo, Russia

Carboxylated phthalocyanines (Pc) attract attention as water-soluble catalysts and photosensitizers, their derivatives can be used for design of liquid-crystalline and electrode materials. Coordination properties of carboxy groups allow assembly of metal-organic frameworks. So far carboxylated phthalocyanines were modified by changing of the central metal or derivatization of carboxyl groups and a series of covalent organic frameworks (COF) with polyimide linkages were prepared for application in photo- and electrocatalysis. Azaanalogues containing instead of benzene rings pyrazine units (TPyzPA) were also synthesized [1,2] and polyimide COF derived therefrom was used as anode materials in potassium ion batteries [3].



Contraction of the central porphyrazine macrocycle present in phthalocyanines and TPyzPA leads tp strong changes in its geometry, coordination and electronic properties. Thus, elimination of one of *meso*-nitrogen atoms leads to corrolazines (CA) and additional exclusion of pyrrole ring to subporphyrazine (sPA), and corresponding phthalocyanine analogues exhibit enhanced photophysical properties. In this presentation we report the synthesis of peripherally carboxylated benzo- and pyrazine fused porphyrazines, phosphorus(V) corrolazines [1,2] and boron(III) subporphyrazines using pyrromelitic and tartaric acids as a cheap precursors. We reveal influence of the macrocycle structure (PA/CA/sPA) and and fused rings (benzene/pyrazine) on the spectral-luminescent, photo- and electrochemical and acid base properties.

The work was carried out with the financial support of the Russian Science Foundation.

REFERENCES

1. Chufarin AE, Skvortsov IA, Lazovskiy DA, Stuzhin PA, *J. Photochem. Photobiol. A*, **2024**, 452, 115564.
2. Lazovskiy DA, Gnedina ES, Nikitin IA, Wang H, Stuzhin PA,.et al. *Inorg. Chim. Acta*, **2026**, 592, 123000.
3. Ding, X.; Zhou, Z.; Chufarin, A. E.; et al *Chem. Engineering J.*, **2025**, *518*, 164913.

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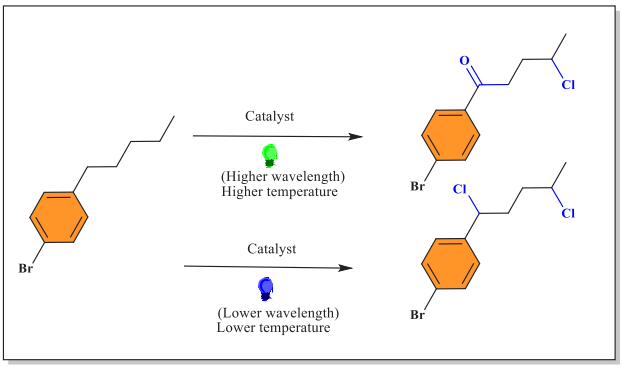
Controlling Bifunctionalisation Pathways in Metalloporphyrin-catalyzed C(sp^3)–H chlorination of Arylalkanes

Nithish Kumar Subramanian[a], Aleksandra Legiecka, Karolina Hurej[a]

[a] *University of Wroclaw, Faculty of Chemistry, F. Joliot-Curie 14, 50-383 Wrocław, e-mail: nithishkumar.subramanian@uwr.edu.pl*

Metalloporphyrins are widely studied as functional molecular systems for promoting alkyl C–H functionalisations, motivated by their structural similarity to enzymatic cofactors and their ability to operate under relatively mild conditions[1]. These complexes have been widely reported to be effective mediators for C(sp^3)–H halogenation [2,3]. While selective bifunctionalisation of the alkyl chain in arylalkane systems is feasible, achieving high selectivity is hindered by parallel activation pathways that yield closely competing products. Following the principle of the previous work on the synthesis of 1,4-dicarbonyl compounds, in which it was hypothesised that water plays a significant role in selectivity [4], this project extends the chlorination protocol.

The role of metalloporphyrin complexes in this transformation under photocatalytic conditions is examined through a comparative, control-based approach. Various *meso*-tetraphenyl-porphyrin complexes incorporating different central metal ions (Mn, Cr, Ti, Co) were evaluated under analogous conditions, alongside reactions performed in the absence of metalloporphyrins. Initial results suggest that product formation is influenced by both the reaction environment and the presence of metalloporphyrin complexes, where slight variations in the reaction parameters alter the functional groups at the carbon centres (Scheme 1). At the same time, control experiments indicate that background reactivity can contribute significantly under certain conditions, highlighting the need for careful interpretation of catalytic effects. Current efforts focus on quantitatively optimising each conditions separately and identifying optimal conditions. GC-MS monitors the reactions and the products are quantitatively analysed by NMR spectroscopy.



Scheme 1. Representation of the slight variation in conditions leading to the two major products in chlorination.

References

1. **Groves, J. T.** *J. Chem. Educ.* **1985**, *62* (11), 928–931.
2. **Liu, W.; Groves, J. T.** *Acc. Chem. Res.* **2015**, *48* (6), 1727–17353.
3. **Li, G.; Dilger, A. K.; Cheng, P. T.; Ewing, W. R.; Groves, J. T.** *Angew. Chem., Int. Ed.* **2018**, *57*, 1251–1255.
4. **Sukiennik, J.; Pranowo, A.; Domański, S.; Hurej, K.** *Chem. Commun.* **2023**, *59*, 1149–1152.

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Halogenated phthalocyanines: Crystal structure, packing motifs, and intermolecular interactions

Aleksandr Sukhikh[a], Darya Klyamer[a], Dmitry Bonegardt[a], Tamara Basova[a]

[a]*Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia*

Metal phthalocyanines have unique physicochemical properties that define a wide range of practical applications as active layers in electronic devices such as solar cells, organic field-effect transistors, and chemical sensors. It is known that the addition of various axial and peripheral substituent atoms to the phthalocyanine ring makes it possible to change the electrophysical, photophysical, and sensory properties of the complex. Among the wide variety of substituents, halogen substituents attract the attention of researchers due to their strong electron-withdrawing character. Another important feature of halogenated phthalocyanines is their relatively good volatility and thermal stability, which allows the growth of single crystals suitable for single-crystal diffraction study by vacuum sublimation. The introduction of peripheral substituents also affects packing motifs of phthalocyanine molecules. Bulky fluorine and chlorine atoms in place of hydrogen atoms change the size and shape of the phthalocyanine molecule, resulting in halogenated phthalocyanines with completely different packing styles and intermolecular contacts compared to their unsubstituted predecessors. Substituent atoms can also be located in peripheral (-p) or non-peripheral (-np) positions, which allows the preparation of halogenated phthalocyanine molecules with the same chemical composition but different crystal structures.

In this study, we compare the packing motifs and intermolecular interactions of various halogen-substituted phthalocyanines $MPcHal_x$ (x = 4, 8, 16; Hal = F, Cl) with their unsubstituted analogs. $MPcHal_x$ exhibit a variety of molecular packing motifs, including molecular stacks, chains, 2D molecular layers, and tetragonal molecular columns. Some halogen-substituted phthalocyanines have multiple polymorph modifications, sometimes with drastically different packing motifs, as in the case of $VOPcCl_4$-p. Since all tetra-substituted $MPcHal_4$ are synthesized as a mixture of regioisomers, halogen atoms in their structures are usually disordered, which sometimes leads to strong halogen-halogen interactions or disordering of the entire phthalocyanine molecule in the case of non-peripherally substituted $MPcCl_4$-np.

Comparison and classification of packing motifs of halogen-substituted phthalocyanines can be useful for the targeted production of crystals and thin films with a given packing motif and intermolecular contacts. We demonstrate that some $MPcHal_x$ can be mixed with unsubstituted MPc, leading to mixed crystalline phases with variable numbers of halogen atoms. In the case of $MPcF_4$-p, their addition to unsubstituted phthalocyanines allows for the forced formation of the triclinic α-phase, which is usually metastable in unsubstituted MPc. The formation of the stable α-phase alters the interactions between molecules in the stack, which in turn affects the physical properties of the resulting mixed phthalocyanine, such as conductivity or sensory response.

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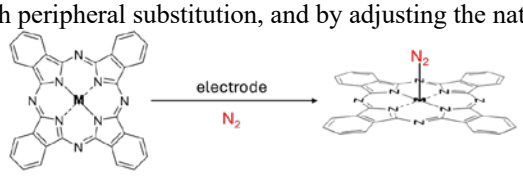
Towards the electrochemical molecular activation of dinitrogen with phthalocyanines

Kenberson Surin[a,b], Dependu Dolui[a], Marc Robert[a,c]

[a]*Sorbonne Université, CNRS, Institut Parisien de Chimie Moléculaire (IPCM), 75005 Paris, France*
[b]*ETSEM Lab, 13790 Rousset, France*
[c]*Institut Universitaire de France (IUF), 75005 Paris, France*

Ammonia (NH_3) synthesis represents a fundamental pillar of the global chemical industry, serving mainly for fertilizer production and, more recently, as a route to hydrogen-based energy carriers. The Haber–Bosch process remains the principal industrial method, enabling the conversion of atmospheric nitrogen (N_2) and hydrogen (H_2) into ammonia [1].
This conversion demands harsh operating conditions, typically 400–500 °C and pressures above 100 bar, owing to the high energy required to cleave the dinitrogen triple bond (941 kJ·mol^{-1}). It consumes approximately 1–3% of the world's electricity and 2–5% of the natural gas supply, resulting in annual CO_2 emissions exceeding 400 Mt.

Metallated phthalocyanines ([M]Pc) recently emerged as a class of potential molecular catalysts for the activation of nitrogen species (nitrate, nitrite but also dinitrogen in some cases) through the combination of their metal center (Fe, Co, Cu, etc.) and their π-conjugated electronic system capable of accumulating charges, the ability to finely modulate their properties through peripheral substitution, and by adjusting the nature of the central metal ion [2].



$N_2 + 6\,H^+ + 6\,e^- \rightleftharpoons 2\,NH_3$

Nevertheless, a major challenge remains the competition with the hydrogen evolution reaction (HER), due to both favorable thermodynamics and kinetics [3].
To limit HER and increase N_2 solubility, we have investigated the use of aprotic and hydrophobic ionic liquids (ILs). Phthalocyanine catalysts with different metals were employed in a three-electrode cell configuration. Our electrochemical and electrolysis experiments in various conditions will be described, and we will also emphasize the necessity for implementing rigorous experimental protocols to avoid false positives and strictly assess the formation of ammonia.

REFERENCES

1. Jia, H.-P.; Quadrelli, E. A. Mechanistic Aspects of Dinitrogen Cleavage and Hydrogenation to Produce Ammonia in Catalysis and Organometallic Chemistry: Relevance of Metal Hydride Bonds and Dihydrogen. Chem. Soc. Rev. 2014, 43 (2), 547–564. https://doi.org/10.1039/C3CS60206K.
2. Xie, L.; Wang, Y.; Kong, Q.; Cao, R. A Minireview on Porphyrin and Phthalocyanine Based Catalysts for Electrocatalytic Synthesis of Ammonia. ChemCatChem 2024, e202400956. https://doi.org/10.1002/cctc.202400956.
3. Tang, C.; Qiao, S.-Z. How to Explore Ambient Electrocatalytic Nitrogen Reduction Reliably and Insightfully. Chem. Soc. Rev. 2019, 48 (12), 3166–3180. https://doi.org/10.1039/C9CS00280D

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Chemical Switching of Aromaticity in N-Confused Porphyrin Complexes

Kinga Szydełko[a], Michał J. Białek[a], Piotr J. Chmielewski[a]

[a] *University of Wrocław, Faculty of Chemistry, F. Joliot-Curie 14,50-383 Wrocław, Poland*

N-confused porphyrin (**NCP**) is an aromatic tetrapyrrole, in which one pyrrole ring is incorporated in the macrocycle with a single β-meso linkage instead of all α-meso bonds, conferring unique coordination properties. **NCP** binds metal ions both within its internal NNNC core and through an external nitrogen donor site, enabling stabilization of diverse metal geometries and oxidation states [1-3]. Reaction of **NCP** with rhodium and iridium complexes in the +III and +I oxidation states affords planar-chiral, aromatic, diamagnetic metal(III) complexes with apically coordinated carbanionic ligands. Addition of molecular iodine induces a pronounced electronic reorganization, yielding a diamagnetic, antiaromatic complex featuring a six-coordinate rhodium(III) center with axial iodide ligands. This represents the first example of **[16]NCP** acting as a tetradentate monoanionic ligand with a 16π-electron perimeter while retaining the +III oxidation state of the metal. An alternative synthetic route involving reaction of M^{III}**NCP**-Ac (M = Ir, Rh) with $K[AuCl_4]$ produces analogous paratropic complexes bearing axial chloride ligands. Overall, **NCP** functions not as a classical donor ligand but as a redox-active, electronically adaptive platform enabling efficient charge delocalization and stabilization of unusual electronic states.

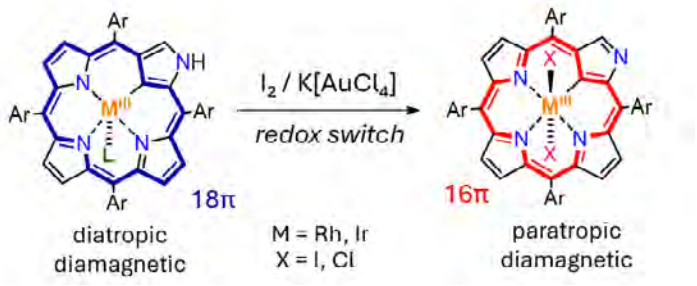


Figure 1. NCP as a redox-adaptive ligand: aromaticity switching

REFERENCES

1. Chmielewski P. J., Latos-Grażyński L., Rachlewicz K., Głowiak T., *Angew. Chem., Int. Ed. Engl.* **1994**, 33, 779.
2. Toganoh M., Furuta H., *Chem.Rev.*, **2022**, 122 , 8313.
2. Srinivasan A., Toganoh M., Niino T., Osuka A., Furuta H., *Inorg. Chem.* **2008**, 47, 11305.

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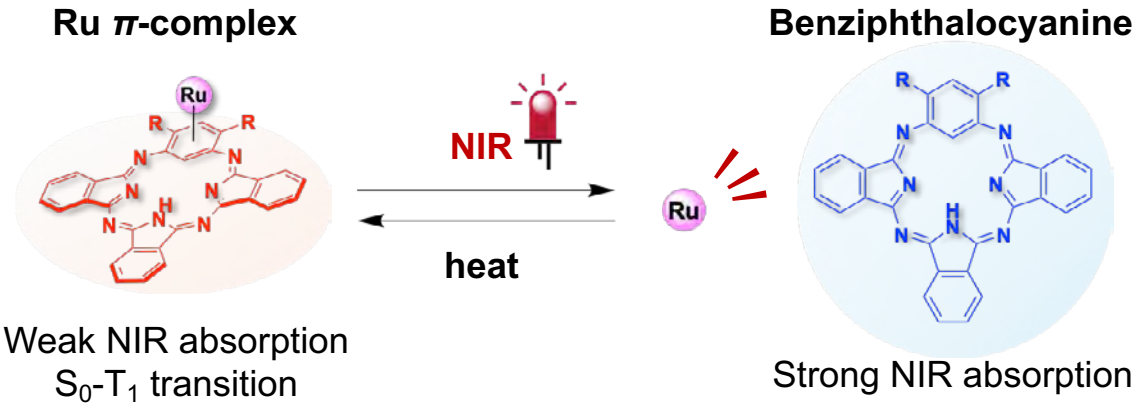


Ruthenium π-arene Complex of Benziphthalocyanine

Orie Takayama[a,b], Naoyuki Toriumi[a], Masanobu Uchiyama[a]

[a]*The University of Tokyo, Graduate School of Pharmaceutical Sciences*
[b]*Keio University, Graduate School of Pharmaceutical Sciences*

The use of near-infrared (NIR) light (700–2000 nm) is highly desirable in life sciences due to its superior tissue transparency, low phototoxicity, and deep tissue penetration. However, most conventional NIR-responsive compounds are activated via S_0-S_1 transitions, which often require relatively high-energy excitation even within the NIR window, resulting in a scarcity of truly effective NIR-active photocages. To address this challenge and extend the excitation wavelength further into the NIR region, we designed and synthesized Ru π-arene complexes of tautomeric benziphthalocyanines (BPcs) [1,2]. Our strategy specifically aims to utilize the low-energy singlet-triplet (S_0-T_1) transition for activation. Experimental characterization, including NMR spectroscopy and single-crystal X-ray diffraction analysis, confirmed that the Ru center selectively coordinates to the benzene ring of the BPc, disrupting the strongly NIR-absorptive, 18π-electron aromatic system of the BPc ligand. Interestingly, theoretical calculations and spectroscopic data indicate that these Ru-BPc complexes still possess weak and broad absorption in the NIR region. This absorption originates from S_0-T_1 transitions with significant metal-to-ligand charge-transfer (MLCT) character. Notably, NIR light irradiation at wavelengths exceeding 800 nm triggered the efficient dissociation of the Ru moiety, releasing the free BPcs and restoring their intense NIR absorption and fluorescence. This mechanism enables a distinct OFF/ON-type activation via NIR-induced Ru release. These results demonstrate the high potential of S_0-T_1 transition-driven Ru-photocages for advanced bioimaging and targeted therapeutic applications.



REFERENCES

1. N. Toriumi, A. Muranaka, K. Hirano, K. Yoshida, D. Hashizume, M. Uchiyama, *Angew. Chem. Int. Ed.* **2014**, *53*, 7814–7818.
2. O. Takayama, N. Toriumi, K. Hanaoka, M. Uchiyama, *submitted*.

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Observation of the phenotypes of mutant lacking the C8-vinyl reductase, BciA or BciB, that is found in the bacteriochlorophyll biosynthesis of photosynthetic bacteria

Jiro Harada[a] and Hitoshi Tamiaki[b]

[a]*Department of Medical Biochemistry, Kurume University School of Medicine, Fukuoka 830-0011, Japan*
[b]*Graduate School of Life Sciences, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan*

In anoxygenic photosynthetic bacteria, six bacteriochlorophyll (BChl) species, BChls *a*, *b*, *c*, *d*, *e*, and *g*, are found, and all of their biosynthetic pathways have been determined [1]. In their synthetic pathways, C8-vinyl reductase (DVR) reduces a vinyl group at the C8 position of divinyl-chlorophyllide *a* to give chlorophyllide *a* (Fig. 1). Among photosynthetic bacteria, there are three types of DVR enzymes, BciA, BciB, and chlorophyllide *a* oxidoreductase (COR) [2]. The phylogenetic analyses for these enzymes showed different phylogenetic trees, suggesting that BciA and BciB evolved later than COR. It is unclear why the BciA and BciB were needed later, despite the presence of COR in photosynthetic bacteria. To answer this question, we constructed DVR mutants of the purple bacteria *Cereibacter sphaeroides* (formerly *Rhodobacter sphaeroides*) and *Rhodopseudomonas palustris,* and analyzed their phenotypes in detail. The results of growth measurements suggested that BciA and BciB play an auxiliary role in pigment synthesis. A *bciA*-deficient strain of the green sulfur bacterium *Chlorobaculum tepidum* was also constructed [3], and we discuss the significance of each DVR enzymes contained in photosynthetic bacteria.

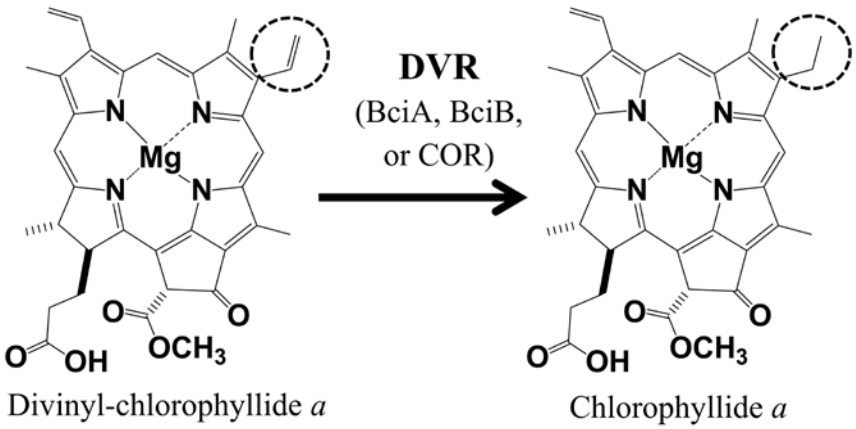


Fig. 1. The reaction of DV-Chlide *a* to Chlide *a* by DVR.

REFERENCES

1. Tamiaki H, Teramura M and Tsukatani Y. *Bull. Chem. Soc. Jpn.* 2016; **89**: 161–173.
2. Harada J, Mizoguchi T, Tsukatani Y, Yokono M, Tanaka A and Tamiaki H. *J. Biol. Chem.* 2014; **289**: 12716–12726.
3. Harada J, Mizoguchi T, Nomura K and Tamiaki H. *Photosynth. Res.* 2014; **121**: 13–23.

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Self-aggregation of synthetic bacteriochlorophyll-*d* analogs with a heptaisobutylated POSS unit in alkane solvents

Sunao Shoji[a,b] **and Hitoshi Tamiaki**[a]

[a]*Graduate School of Life Sciences, Ritsumeikan University, Noji-higashi 1-1-1, Kusatsu, Shiga 525-8577, Japan*
[b]*Faculty of Engineering, Nara Women's University, Kitauoya-Nishimachi, Nara, Nara 630-8506, Japan*

Chlorosomes are major light-harvesting antenna systems in green photosynthetic bacteria, in which bacteriochlorophyll(BChl)-*c*, *d*, and *e* pigments self-aggregate into *J*-aggregates in hydrophobic environments through coordination bonding, hydrogen bonding, and π-π stacking interactions. Synthetic analogs of these pigments have been prepared to elucidate the detailed mechanism of chlorosomal self-aggregation [1,2]. Reproducing such chlorosomal self-aggregation in simple nonpolar organic media remains challenging because BChls-*c*–*e* pigments and their analogs are poorly dispersible in neat alkane solvents.

In this study, we demonstrate chlorosomal self-aggregation of zinc BChl-*d* analogs in single-alkane solvents by introducing a highly hydrophobic heptaisobutylated polyhedral oligomeric silsesquioxane (POSS) moiety in the 17-substituent. Ester- and amide-type POSS-linked BChl-*d* analogs (**Zn-Chl-POSS-E** and **Zn-Chl-POSS-A**) were synthesized (Fig. 1, left) [3], and their self-aggregation behavior was investigated in neat alkane solvents, including *n*-hexane, cyclohexane, isooctane, *n*-octane, and *n*-decane, using spectroscopic techniques. In the single-alkane solvents, both the analogs formed homogeneous chlorosomal *J*-aggregates rather than monomeric species (Fig. 1, right). After heat treatment of the dispersed solutions, well-defined chlorosomal self-aggregates were obtained, particularly in *n*-decane. Thermal stability measurements further revealed higher robustness for the self-aggregates of **Zn-Chl-POSS-A**. These results indicate that the POSS unit functions not only as a hydrophobic solubilizing group but also as a steric regulator of supramolecular organization, providing a new strategy for constructing chlorophyll-based light-harvesting assemblies in simple nonpolar environments.

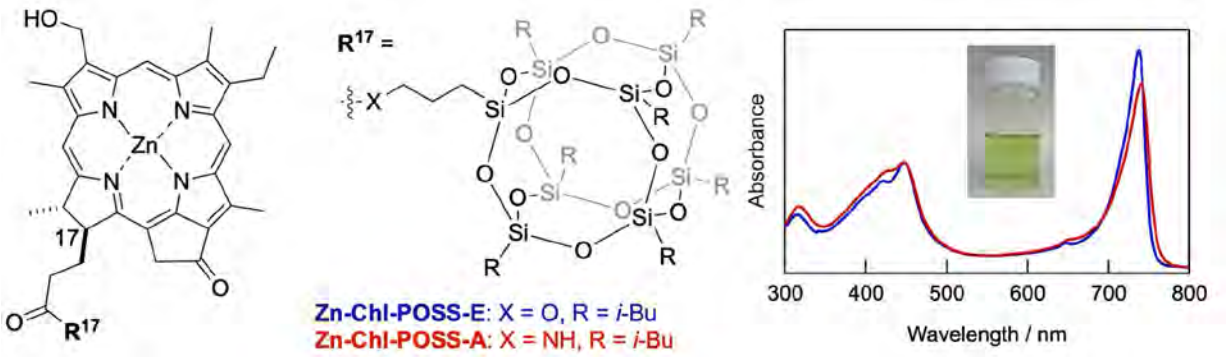


Fig. 1. Molecular structures of BChl-*d* analogs **Zn-Chl-POSS-E/A** (left) and their electronic absorption spectra in *n*-octane (right).

REFERENCES

1. S. Matsubara, H. Tamiaki, *J. Photochem. Photobiol. C: Photochem. Rev.*, **45**, 100385 (2020).
2. S. Matsubara, S. Shoji, H. Tamiaki, *Chem. Commun.*, **60**, 12513 (2024).
3. S. Shoji, H. Idei, T. Nakano, H. Tamiaki, *Chem. Lett.*, **55**, upag001 (2026).

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Metal-driven Dimerization of Porphyrins bearing Bipyridine Ligands Modified with Ethylene Glycol Chains

Kota Taniguchi[a], Tomoya Abe[a], Yuto Nakaie[a], Ryota Yamada[a], Masaya Domyo[a], Ayumu Murokoshi[a], Yousuke Hosoya[a], Kosuke Sugawa[a], and Joe Otsuki[a]

[a]*College of Science and Technology, Nihon University*

We have previously demonstrated that the addition of Zn^{2+} ions to porphyrins bearing peripheral bipyridine (ZnPor(bpy)$_4$) [1] or phenanthroline ligands [2] induces highly cooperative face-to-face dimerization (Figure 1). These dimers exhibit a well-defined 2:4 porphyrin–metal stoichiometry and strong positive cooperativity in the dimerization process. However, the ZnPor(bpy)$_4$ dimer exhibits limited solubility even in organic solvents, let alone in water. To address this limitation, we introduced oligoethylene glycol (OEG) chains onto the bipyridine ligands to design ZnPor(bpyEG*n*)$_4$ (*n* = 3, 7; Figure 2). These compounds were synthesized by first functionalizing the bipyridine unit with an EG*n* chain, followed by conjugation to a tetraphenylporphyrin core bearing Bpin groups at the 3-positions of the meso-phenyl rings.

Addition of Zn^{2+} to ZnPor(bpyEG3)$_4$ resulted in UV–vis and ^{1}H NMR spectral changes that closely resemble those of the parent ZnPor(bpy)$_4$ system. Furthermore, titration of ZnPor(bpyEG3)$_4$ with Zn(OTf)$_2$ produced an S-shaped binding curve with 1:2 saturation behavior, again similar to that of ZnPor(bpy)$_4$. These results indicate that introduction of OEG chains preserves the cooperative metal-driven dimerization motif and the overall dimer structure. The modified dimers exhibit enhanced solubility. Whereas a 0.5 mM solution of the ZnPor(bpy)$_4$ dimer with Zn(OTf)$_2$ does not dissolve in CH_3CN, the corresponding ZnPor(bpyEG3)$_4$ dimer (0.5 mM) is soluble in CH_3CN. These findings demonstrate that OEG functionalization retains cooperative metal-driven porphyrin dimerization while improving solubility, providing a promising platform for the development of supramolecular porphyrin catalysts operable in polar environments.

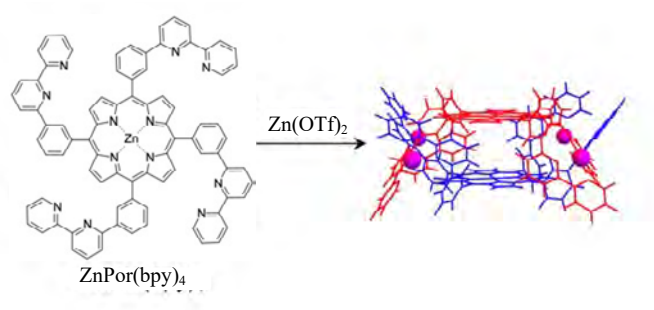


Figure 1. Self-assembly into a face-to-face dimer of a porphyrin with four bipyridine sites upon addition of Zn(OTf)$_2$ [1].



Figure 2. ZnPor(bpyEG*n*)$_4$ (*n* = 3, 7).

REFERENCES

1. J. Otsuki *et al., Eur. J. Inorg. Chem*., **2024**, *27*, e202400188.
2. J. Otsuki *et al*., *Chem. Lett.*, **2025**, *54*, upaf182.

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POSTERS



1000 Absorption and fluorescence spectra of tetrapyrroles – collected with friends and chatbots for PhotochemCAD

Masahiko Taniguchi and Jonathan S. Lindsey

Department of Chemistry, North Carolina State University, Raleigh, NC 27695 USA

The characteristic colors of tetrapyrrole macrocycles – the pigments of life – make absorption spectroscopy a first method of analysis. Over the years, we have been collecting spectra for precious compounds in this class (both synthetic and natural), including bacteriochlorins, chlorins, dipyrrins, phthalocyanines, phyllobilins, and porphyrins. Other databases focus on betaxanthins, carotenoids, chlorophylls (at low temperature), common compounds, and flavonoids. The spectra – curated with accompanying photophysical parameters (molar absorption coefficient, fluorescence quantum yield) and ties to the original scientific literature – have been assembled and made freely available in PhotochemCAD (www.photochemcad.com).

We are currently working to create new databases and make all of the spectra available via a Smartphone app. The creation of databases – while often painstaking – may be enabled to some extent by the use of chatbots [1], but friends make the best collaborators. The references listed below stem from collaborations with the groups of Williams [2], Karg and Moser [3], Bastos [4], and Niedzwiedzki [5]. We also seek collaborations with others who have spectra of members of the fascinating tetrapyrrole family of compounds.

This research is supported in part by the NSF (CHE-2348052).

REFERENCES

1. "Acquisition of Absorption and Fluorescence Spectral Data Using Chatbots," Taniguchi, M.; Lindsey, J. S. *Digit. Discov.* **2025**, *4*, 21–34.
2. "Tolyporphins A–R, Unusual Tetrapyrrole Macrocycles in a Cyanobacterium from Micronesia, Assessed Quantitatively from the Culture HT-58-2," O'Donnell, T. J.; Gurr, J. R.; Dai, J.; Taniguchi, M.; Williams, P. G.; Lindsey, J. S. *New J. Chem.* **2021**, *45*, 11481–11494.
3. "Phyllobilins – Bioactive Natural Products Derived from Chlorophyll – Plant Origins, Structures, Absorption Spectra, and Biomedical Properties," Karg, C. A.; Taniguchi, M.; Lindsey, J. S.; Moser, S. *Planta Med.* **2023**, *89*, 637–662.
4. "Amino Acid Betaxanthins: Absorption, Fluorescence, and Stability," Esteves, L. C.; Pinheiro, A. C.; Machado, C. O.; Taniguchi, M.; Lindsey, J. S.; Bastos, E. L. *J. Nat. Prod.* **2025**, *88*, 2301–2312.
5. "Database of Low-Temperature Electronic Spectra of Native Photosynthetic Tetrapyrrole Macrocycles," Niedzwiedzki, D. M.; Taniguchi, M.; Lindsey, J. S. *Photochem. Photobiol.* **2026**, DOI: 10.1111/php.70018.

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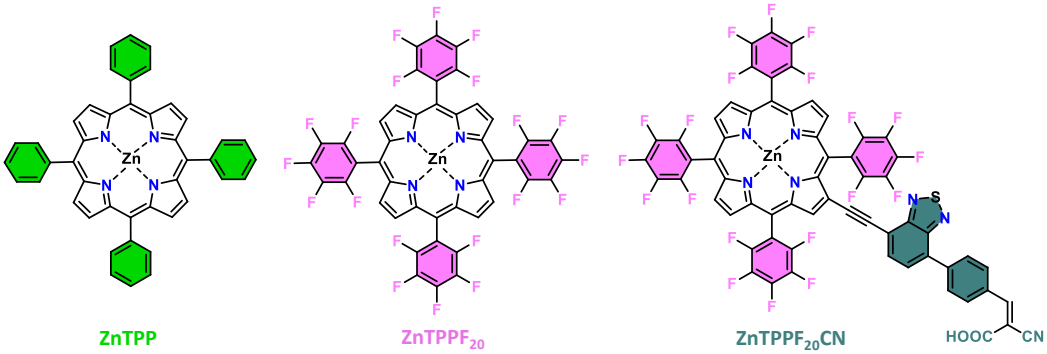


Interplay Between SnO_2 and Perfluorinated Zn(II) Porphyrins: Electronic Effects and Chemisorption–Physisorption Mechanisms in Acetone Chemiresistive Detection

Francesca Tessore[a], Giuseppe Cappelletti[a], Gian Luca Chiarello[a], Gabriele Di Carlo[a], Manuel Minnucci[a], Sara Oregioni[a], Rocco Martinazzo[a]

[a] *Department of Chemistry, University of Milan, via Golgi 19 20133 Milan (Italy)*

SnO_2 nanoparticles were hybridized with three Zn(II) porphyrins (physisorbed ZnTPP and its perfluorinated analogue $ZnTPPF_{20}$, and chemisorbed $ZnTPPF_{20}CN$) to investigate how porphyrin chemistry and anchoring modes may influence acetone chemiresistive sensing at 120 °C.



Hybrid materials with 1:4, 1:32, and 1:64 porphyrin/SnO_2 weight ratios were evaluated under dark conditions and LED illumination. For physisorbed systems, $ZnTPPF_{20}/SnO_2$ at a 1:32 ratio achieved the best performance, including a 200 ppb detection limit, correlating with an optimal balance between electron injection and the availability of SnO_2 electronic states. DFT calculations confirmed electron donation from ZnTPP and $ZnTPPF_{20}$ to the SnO_2 conduction band, with excessive injection leading to electronic saturation and reduced sensing efficiency [1]. The chemisorbing $ZnTPPF_{20}CN$ derivative, designed with an ethynylphenyl-cyanoacrylic anchoring group and a benzothiadiazole spacer, enabled stronger interfacial coupling. Despite lower intrinsic conductivity, the 1:32 $ZnTPPF_{20}CN/SnO_2$ hybrid outperformed its physisorbed $ZnTPPF_{20}/SnO_2$counterpart, benefiting from a more favorable charge-injection/surface-state balance [2].
LED illumination showed no improvement due to porphyrin-related electronic scattering. These results highlight how molecular engineering and optimized loading ratios can tailor charge dynamics and boost the performance of porphyrin/SnO_2 chemiresistive acetone sensors.

REFERENCES

1. Tessore, F. ; Pargoletti, E. ; Di Carlo, G. ; Albanese, C. ; Soave, R. ; Trioni, M.I. ; Marelli, F. ; Cappelletti, G. *ACS Appl. Mater. Interfaces* **2024**, *16*, 41086.
2. Minnucci, M. ; Oregioni, S. ; Pargoletti, E. ; Di Carlo, G. ; Tessore, F. ; Chiarello, G.L. ; Martinazzo, R. ; Trioni, M.I. ; Cappelletti, G. *Molecules* **2025**, *30*, 4749.

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Integrating Twisted and Push-Pull Structural Motifs for Efficient Dual-Functioning Near-Infrared BODIPY Photosensitizers

Nele Theysmans[a,b], Mathias Fraiponts[a,b,c], Greta Sambucari[d], Thomas Leendertse[b,e], Alessia Pancaro[b,e,f], Lisa Reynders[a], Jasper Deckers[a,b], Barbara Patrizi[g], Kristof Van Hecke[h], Laurence Lutsen[a,b], Anitha Ethirajan[b,e], Mariangela di Donato[d,i], Benoît Champagne[c], Wouter Maes[a,b]

[a] *UHasselt, Institute for Materials Research (IUMAT), Design & Synthesis of Organic Semiconductors (DSOS), Martelarenlaan 42, B-3500 Hasselt, Belgium*
[b] *Imec, IUMAT, Wetenschapspark 1, B-3590 Diepenbeek, Belgium*
[c] *University of Namur, Laboratory of Theoretical Chemistry (LTC), Theoretical and Structural Physical Chemistry Unit, Namur Institute of Structured Matter, Rue de Bruxelles 61, B-5000 Namur, Belgium*
[d] *LENS - European Laboratory for Non Linear Spectroscopy, via N. Carrara 1, 50019 Sesto Fiorentino (FI), Italy*
[e] *UHasselt, Institute for Materials Research (IUMAT), Nanobiophysics and Soft Matter Interfaces (NSI), Martelarenlaan 42, B-3500 Hasselt, Belgium*
[f] *Flemish Institute for Technological Research (VITO) Environmental Intelligence Unit Boeretang 200, Mol 2400, Belgium*
[g] *CNR-INO, via N. Carrara 1, 50019 Sesto Fiorentino (FI), Italy*
[h] *XStruct, Ghent University, Department of Chemistry, Krijgslaan 281-S3, B-9000 Ghent, Belgium*
[i] *Instituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), Via Madonna Del Piano 10, 50019 Sesto Fiorentino (FI), Italy*

Developing organic photosensitizers that efficiently combine fluorescence with singlet oxygen generation remains a significant challenge toward image-guided photodynamic therapy, as these pathways compete for the same excited-state population. While BODIPY dyes are generally limited by poor intersystem crossing (ISC), the implementation of twist-induced or spin-orbit charge-transfer (SOCT) ISC provides heavy-atom-free alternatives to facilitate triplet-state formation. In this work, the twisted BODIPY core reported by Dong *et al.* was selected as a scaffold because of its favorable balance between fluorescence and singlet oxygen quantum yield.[1] To extend the absorption and emission into the phototherapeutic window (600–800 nm), the BODIPY core was functionalized *via* a Knoevenagel condensation to introduce various electron-donating moieties, enabling SOCT ISC.[2] By integrating these twist-induced and SOCT ISC strategies into a single framework, we aimed to achieve high-performance, dual-functioning photosensitizers. The resulting structure-property relationships, supported by quantum-chemical calculations and transient absorption spectroscopy, elucidate the role of the charge-transfer state in mediating efficient ISC. We demonstrate that by tuning the electronic nature of the substituents, a favorable balance between singlet oxygen quantum yield and fluorescence can be achieved. To bridge the gap to therapeutic application, we also present preliminary *in vitro* assays evaluating the biocompatibility and photo-induced cytotoxicity of the most promising BODIPY dyad in cancer cell lines.

REFERENCES

1. Y. Dong, B. Dick and J. Zhao, Org. Lett., **2020**, *22*, 5535.
2. J. Deckers, T. Cardeynaels, H. Penxten, A. Ethirajan, M. Ameloot, M. Kruk, B. Champagne and W. Maes, Chem. Eur. J., **2020**, *26*, 15212.

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Single Molecular Conductance of Antiaromatic 5,15-Dioxaporphyrin and Its Quantum Interferences

Taiyou Tsutsumi, Yukako Kawashige, Takanori Iwasaki, Soji Shimizu

Department of Applied Chemistry, Graduate School of Engineering, Kyushu University, Fukuoka 819-0395, Japan (tsutsumi.taiyou.042@s.kyushu-u.ac.jp)

Antiaromatic compounds are expected to exhibit prominent charge-transport properties because of their narrow HOMO–LUMO gaps. However, their conductive properties both in bulk and at the single molecular level have been elusive because suitably stable antiaromatic compounds for these investigations have been scarce.[1] In addition, to elucidate single-molecular conductance, the quantum interference (QI) of electron waves passing through different pathways in macrocyclic systems should be taken into account. There are two types of QI, constructive and destructive, arising from in-phase and out-of-phase interferences, respectively, which are determined by the phases of the HOMO and LUMO at the linking positions to the electrodes.[2]

Recently, we reported 5,15-dioxaporphyrin (DOP) as a stable 20π antiaromatic molecule[3] and developed functionalization reactions at the peripheral positions. These reactions enable the incorporation of anchoring groups at various positions for single-molecule conductance studies using the STM break-junction (STM-BJ) method.

In this study, we synthesized DOP derivatives bearing two 4-aminophenylethynyl anchor groups at the 3,13- and 3,17-positions (**3,13-DOP** and **3,17-DOP**), corresponding to DQI and CQI pathways, respectively, as predicted by first-principles calculations.

In the synthesis of **3,13-DOP** and **3,17-DOP**, **3,13-2Br-DOP** and **3,17-2Br-DOP** were prepared from the nickel complexes of **3Br-dipyrromethene (DPM)** or **2Br-DPM** and **4Br-DPM**. Because the bromination of DPM was difficult to control and the brominated species could not be isolated due to their similar polarities, the mixture was directly subjected to Sonogashira couplingAfter the introduction of the 4-aminophenylethynyl substituents, **3,13-DOP** and **3,17-DOP** were successfully separated by silica gel column chromatography owing to the polarity differences. The STM-BJ measurements revealed that the single molecular conductance of **3,13-DOP** is approximately one order of magnitude higher than that of **3,17-DOP**. The transmission spectra obtained by fixing the working potential in STM-BJ measurements under electrochemical control showed significantly lower conductance for **3,13-DOP** than for **3,17-DOP**, indicating stronger suppression of charge transport due to destructive quantum interference (DQI). **3,13-DOP** also exhibited an abrupt change in conductance with an on/off ratio exceeding two orders of magnitude. Full-range potential-scan measurements of **3,13-DOP** were performed while maintaining the single molecular junction and fixing bias voltage, revealing that the antiresonance dip was too deep to be detected.



In this presentation, we will report in detail on these results and generalize the single molecular conductance of antiaromatic species.

REFERENCES

1. S. Fujii, S. Marqués-González, J. Shin, H. Shinokubo, T. Masuda, T. Nishino, N. P. Arasu, H. Vázquez, M. Kiguchi, *Nat. Commun.* 2017; 8: 15984.
2. K. Yoshizawa, *Acc. Chem. Res.* 2012; 45: 1612.
3. A. Nishiyama, M. Fukuda, S. Mori, K. Furukawa, H. Fliegl, H. Furuta, S. Shimizu, *Angew. Chem. Int. Ed.* 2018;

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The Cytochrome *c* Oxidase -Y280H, -W272H and -Y167F/O_2/H_2O_2 Reactions by UV-Raman Spectroscopy

Constantinos Varotsis [a], Takehiro Ohta[b], Kerstin Budiman[c], Oliver-Matthias H. Richter[d], Teizo Kitagawa[b], Bernd Ludwig[d] and Eftychia Pinakoulaki[e]

[a]*Department of Chemical Engineering, Cyprus University of Technology, 3603 Limassol, Cyprus*
[b]*Okazaki Institute for Integrative Bioscience, National Institutes of Natural Sciences 5-1 Higashiyama, Myodaiji, Okazaki, Aichi 444-8787 Japan*
[c]*Max-Planck Institut für Biophysik, D-60439 Frankfurt am Main, Germany*
[d]*Institute of Biochemistry, Biozentrum, Johann Wolfgang Goethe-Universität, Marie-Curie-Str. 9, D-60439 Frankfurt/M., Germany*
[e]*Department of Chemistry, University of Cyprus, 2109 Aglantzia, Cyprus*

In cell respiration, tyrosyl radicals play a crucial role in the formation of ferry intermediates which are stabilized for efficient energy conservation and proton translocation. The properties of the P and F ferryl intermediates in the reactions of oxidized cytochrome *c* oxidase (CcO) from *P. denitrificans* with H_2O_2 were investigated by monitoring the 244-nm resonance Raman spectra of tyrosine-280, tyrosine-167 and tryptophan-267 mutants. At early times in the reaction, the RR spectra of the reactions of Tyrosine-280 and wild type are nearly identical and showed the formation of bands characteristic of tyrosine/tyrosinate and tryptophan residues. The decay of these transient species to the oxidized form of the enzyme is completed within 15 minutes after mixing with H_2O_2. The reaction of MV CcO Y280 with O_2 was also investigated by Uv-Raman spectroscopy. The time evolution of the transient species formed will be presented.

REFERENCES

1. E. Pinakoulaki, V. Daskalakis, T. Ohta, O-H Richter, K. Budiman, T. Kitagawa, B. Ludwig, C. Varotsis, The protein effect in the structure of two ferryl-oxo intermediates at the same oxidation level in the heme copper binuclear center of cytochrome *c* oxidase, *J. Biol. Chem.*, 288 (2013) 20261-20266.
2. V. Daskalakis, S.C. Farantos, C. Varotsis, Assigning vibrational spectra of ferryl–oxo intermediates of cytochrome *c* oxidase by periodic orbits and molecular dynamics, *J. Am. Chem. Soc.*, 130 (2008) 12385–12393.
3. E. Pinakoulaki, V. Daskalakis, C. Varotsis, The origin of the FeIV=O intermediates in cytochrome aa_3 oxidase *Biochimica et Biophysica Acta (BBA)-Bioenergetics*, 1817 (2012**)** 552-557.

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A spectroscopic and computational analysis of the interaction of a porphyrinic cage with ethionamide

Federica Ruani[a], Sonia Adrouche[b], Gianluca Dell'Orletta[c], Daniel Sánchez-Resa[a], Andrea Barbieri[a], Stéphanie Durot[b], Isabella Daidone[c], Valérie Heitz[b], Nicola Armaroli,[a] Barbara Ventura[a]

[a]*Istituto per la Sintesi Organica e la Fotoreattività (ISOF), Consiglio Nazionale delle Ricerche (CNR), Via P. Gobetti 101, 40129 Bologna, Italy.*
[b]*Laboratoire de Synthèse des Assemblages Moléculaires Multifonctionnels, Institut de Chimie de Strasbourg, CNRS/UMR 7177, Université de Strasbourg, 4 rue Blaise Pascal, 67000 Strasbourg, France.*
[c]*Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, via Vetoio (Coppito 1), 67100 L'Aquila, Italy.*

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A covalent porphyrinic cage consisting of two free-base porphyrins linked by four ethylene glycol–based triazole pillars was designed as a chemically responsive host. Interestingly, coordination of Ag(I) ions to the lateral triazole units locks the cage in an open conformation [1].
The interaction of the open form of the cage with ethionamide (ETH), a biologically active molecule, was investigated by steady-state and time-resolved optical spectroscopies. ETH induces pronounced changes in the absorption and emission features of the porphyrinic cage, indicating a strong interaction with the cage structure. Using a combined spectroscopic and computational approach, including ultrafast transient absorption spectroscopy, NMR studies, quantum-mechanical calculations, and molecular dynamics simulations, we demonstrated that two ETH molecules selectively bind and remove two Ag(I) ions from the cage. This partial metal decoordination induces a conformational transition to a semi-closed, V-shaped structure with a reduced interporphyrinic distance (Fig. 1) [2]. These results highlight the ability of cage structures with multiple binding sites to serve as probes for biomolecules or drugs, enabling their detection via precise spectroscopic signatures.

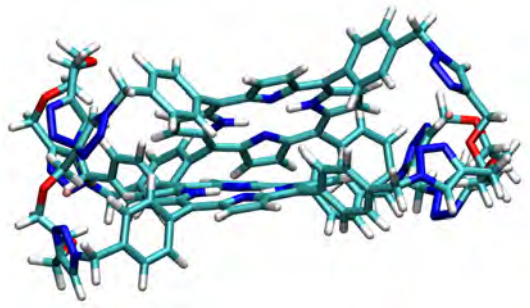


Fig. 1: Optimized structure of the cage with two residual Ag(I) ions at the QM level including solvent effects (CPCM), showing a pronounced V-shaped geometry resulting from the removal of two Ag(I) ions.

Acknowledgement. The projects "CNR-Light-Induced Processes (LIP)" and H2020-MSCA-ITN-2017-765297-NOAH are acknowledged.

REFERENCES

1. D. Sánchez-Resa, I. Daidone, R. Djemili, S. Adrouche, S. Durot, V. Heitz, L. Zanetti-Polzi, B. Ventura *J. Phys. Chem. B* **2022**, *126*, 3450-3459.
2. F. Ruani, S. Adrouche, G. Dell'Orletta, D. Sánchez-Resa, A. Barbieri, S. Durot, I. Daidone, V. Heitz, N. Armaroli, B. Ventura *Photochem. Photobiol. Sci.* **2026** *Accepted*

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Photoinduced processes in Ru(bpy)$_3$-porphyrin dyads designed for carbon dioxide valorization

Alejandra Saavedra Moncada, Elisa Bandini, Marco Agnes, Andrea Barbieri, Nicola Armaroli, Barbara Ventura

Istituto per la Sintesi Organica e la Fotoreattività (ISOF), Consiglio Nazionale delle Ricerche (CNR), Via P. Gobetti 101, 40129 Bologna, Italy.

The conversion of CO_2 into fuels or chemicals with high energy content is an important strategy for mitigating climate change by using carbon-based energy vectors [1]. In this view, it is important to develop efficient catalysts and methodologies for the conversion of CO_2 through green, renewable, and sustainable chemical approaches, employing electrochemical, photochemical, and photoelectrochemical methods [2].
In collaboration with the Universities of Milan and Turin, we developed and screened a series of dyads composed by a porphyrin unit, acting as catalyst, and a Ru(II)-polypyridine complex, serving as photosensitizer. The explored porphyrin units were either free-base or metalated with Zn(II), Cu(II) or Co(II) (Figure 1).

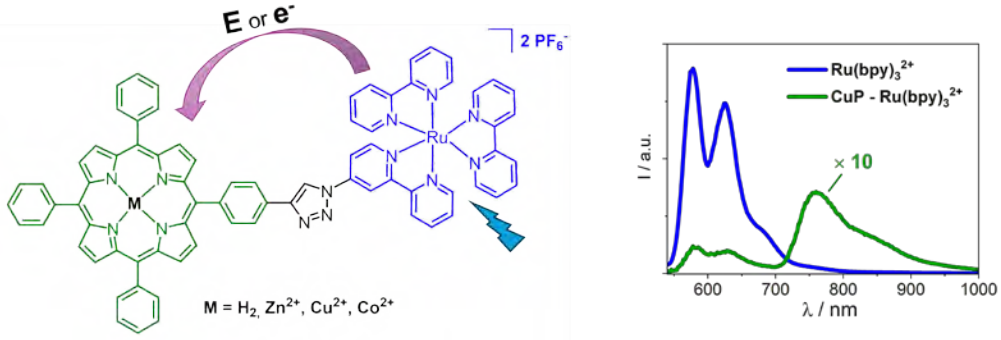


Figure 1. Chemical structures of the studied dyads and sketch of the possible photoinduced processes (left). Emission spectra at 77K of Ru(bpy)$_3^{2+}$ model and dyad CuP-Ru(bpy)$_3^{2+}$ (right).

Here, we report on the photophysical characterization of these dyads, with reference to their corresponding model systems. Steady-state investigations and ultrafast transient absorption studies allowed to elucidate the photoinduced processes occurring among the two units in the dyads and to evaluate their potential as photocatalytic systems.

This research was partially funded by the European Union – NextGeneration EU NRRP M4, C2, I1.1 MUR–PRIN 2022FWAF2M "CADIVAPE", CUP B53D23013670006, and Ecosistema ECOSISTER –Ecosystem for Sustainable Transition in Emilia-Romagna (codice ECS00000033) funded PNRR, M 4, C 2, I 1.5, Creazione e rafforzamento di "Ecosistemi dell'innovazione", CUP B89I22000650001.

REFERENCES

1. C. Fu, Z. Wan, X. Yang, J. Zhang, Z. Zhang *J. Mater. Chem. A*, **2024**, *12*, 28618–28657.
2. M. Tahir, A. Shah, M. Javed, R. Khalida, F. Jan Iftikhar *Catal. Sci. Technol.*, **2026**, Advance Article DOI: 10.1039/D5CY01193K

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Influence of Molecular Rotation on the Stability of Charge-Separated State in Non-Fullerene Supramolecular Assemblies

Victoria Villarreal,[a] Andrew Healy,[b] Rachel Swedin,[b] Michael D. Gutierrez,[a] David Blank,[b] and Victor N. Nemykin[a]

[a] *Department of Chemistry, University of Tennessee – Knoxville, TN, USA (vvillarr@vols.utk.edu)*
[b] *Department of Chemistry, University of Minnesota – Minneapolis, MN, USA*

Previously, the preparation and optical properties of a series of viscosity-sensitive molecular rotor BODIPYs were reported.[1] The fluorescence lifetime of the molecular rotor BODIPYs was drastically increased by increasing the viscosity of the solution, which inhibited twisted intramolecular charge transfer (TICT). In the present study, we propose the preparation of a novel molecular rotor BODIPY electron acceptor bearing a meso-isoxazolyl unit and terminal pyridine substituents. The novel molecular rotor BODIPY acceptor will be characterized using 1H-NMR, high-resolution mass spectrometry (HRMS), single-crystal X-Ray diffraction (XRD), and electrochemical methods, and its optical properties will be investigated using static and time-resolved absorption and emission in viscous and non-viscous environments. Subsequently, the effect of meso-isoxazolyl rotation on the stability of the charge-separated (CS) state following photoinduced electron transfer (PET) in the resultant non-covalent supramolecular assemblies, formed via nitrogen lone pair axial-coordination to zinc porphyrinoid electron donor, will be investigated using time-resolved absorption and emission spectroscopies measured in viscous and non-viscous solvents.

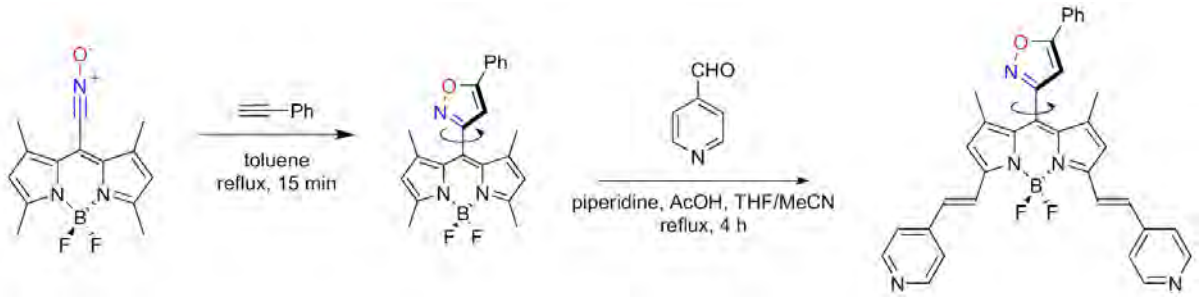


Figure 1. Synthetic scheme for the proposed novel molecular rotor BODIPY.

REFERENCES

1. Zatsikha, Y. V.; Didukh, N. O.; Swedin, R. K.; Yakubovskyi, V. P.; Blesener, T. S.; Healy, A. T.; Herbert, D. E.; Blank, D. A.; Nemykin, V. N.; Kovtun, Y. P. Preparation of Viscosity-Sensitive Isoxazoline/Isoxazolyl-Based Molecular Rotors and Directly Linked BODIPY–Fulleroisoxazoline from the Stable *Meso*-(Nitrile Oxide)-Substituted BODIPY. *Org. Lett.* **2019**, *21* (14), 5713–5718.

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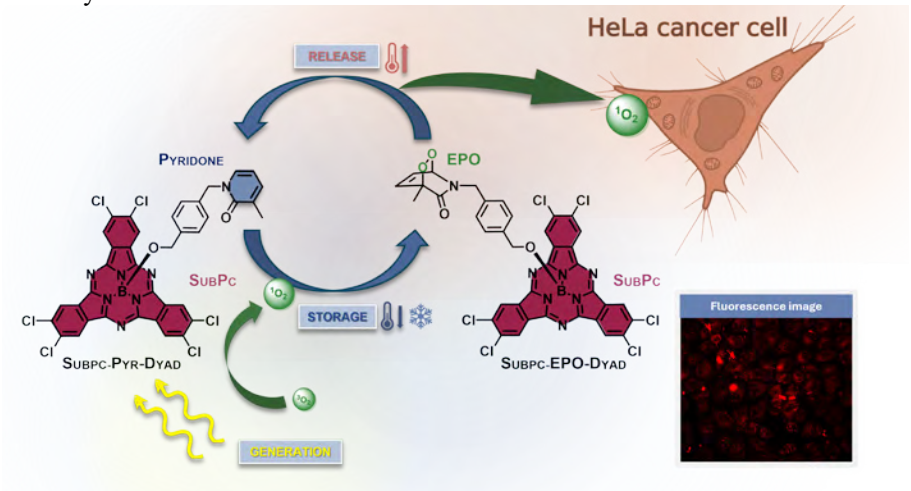
Thermally Controlled Singlet Oxygen Storage and Release from a SubPc-Pyr-Dyad in HeLa Cells

Lorena Vogt[a], **Anika Petersen**[a], **Valeska Viereck**[b], **Frank Abendroth**[b], **Olalla Vázquez**[b] **and Rüdiger Faust**[a]

[a]*University of Kassel, Institute for Chemistry and CINSat – Center for Interdisciplinary Nanostructure Science and Technology, Heinrich-Plett-Straße 40, 34132 Kassel, Germany. (r.faust@uni-kassel.de)*
[b]*Philipps-University Marburg, Department of Chemistry, Hans-Meerwein-Straße 4, 35043 Marburg, Germany (olalla.vazquez@staff.uni-marburg.de)*

The cycloaddition of singlet oxygen ($^1O_2$) to pyridones leads to the formation of endoperoxides (EPOs), enabling the reversible storage of $^1O_2$ as well as its controlled, time-delayed, thermally triggered release via a cycloreversion process.[1] Owing to this property, EPOs represent a promising alternative to conventional photosensitizers in photomedical applications, as they have the potential to overcome limitations associated with tumor hypoxia.[2,3] The release of $^1O_2$ from EPOs occurs with regeneration of the parent compound, rendering the storage process inherently reversible and repeatable.[1-3]

Herein, we report a dyadic system based on a pyridone-functionalized subphthalocyanine (SubPc) scaffold. The dyad acts as an efficient $^1O_2$ photosensitizer within the region of its absorption maximum and simultaneously enables the storage of SubPc-generated $^1O_2$ in the form of pyridone-centered endoperoxides. The reversibility of this process was thoroughly investigated by photophysical, photochemical, and NMR spectroscopic methods. In addition, the functionality of the dyad was evaluated in aqueous media. Cellular uptake in HeLa cancer cells was examined by fluorescence microscopy, and the photodynamic activity in HeLa cells was assessed using dark/light cycles in an MTT assay.



REFERENCES

1. M. Matsumoto, M. Yamada, N. Watanabe, *Chem. Commun.* **2005**, *4*, 483-485.
2. M.A. Filatov, M.O. Senge, *Mol. Syst. Des. Eng.* **2016**, *1*, 258-272.
3. I.S. Turan, D. Yildiz, A. Turksoy, G. Gunaydin and E.U. Akkaya, *Angew. Chem.* **2016**, *128*, 2925-2928.

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Epidermal Growth Factor Receptor-Mediated Double-Gated Bioorthogonal Activation of Photosensitizers for Targeted Photodynamic Therapy

Shuai Wang, Qingshuang Zou, and Dennis K. P. Ng*

Department of Chemistry, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China

Precise delivery and activation of photosensitizers represent a pivotal paradigm for targeted photodynamic therapy (PDT), which can enhance the treatment efficacy and reduce the unwanted side effects [1]. While tremendous efforts have been devoted to achieving these goals, the outcome is still suboptimal mainly due to the high heterogeneity of the tumor microenvironment. As part of our continuing effort in this endeavor [2], we report herein a double-gated bioorthogonal activation approach using epidermal growth factor receptor (EGFR) as the target. It involves the use of a tetrazine-modified erlotinib analogue (Erlo-Tz) that can bind the EGFR overexpressed in cancer cells. The tetrazine moiety also serves as an activator of a distyryl boron dipyrromethene-based photosensitizer substituted with a *trans*-cyclooctene (TCO)-caged ester group and an EGFR-binding peptide, which also promotes the cellular uptake of the compound into EGFR-overexpressed cancer cells. Hence, the EGFR serves as a gate to promote the localization of the two components in target cancer cells where the tetrazine and TCO moieties undergo an inverse electron-demand Diels-Alder reaction to trigger the activation of the photosensitizer. Notably, Erlo-Tz concurrently inhibits EGFR autophosphorylation and synergizes the photodynamic action, leading to effecitve elimination of the cancer cells and suppressing the tumor growth in a 4T1 tumor-bearing mouse model. This combined strategy also induces persistent EGFR downregulation, thereby potentially mitigating the drug resistance issue of conventional tyrosine kinase inhibitors [3]. Collectively, this double-gated bioorthogonal activation approach establishes a therapeutic blueprint for precise and synergistic PDT against cancer.

This work was supported by a Collaborative Research Fund from the Research Grants Council of the Hong Kong Special Administrative Region, China (ref. no. C4057-24GF).

REFERENCES

1. Huis in't Veld, R. V.; Heuts, J.; Ma, S.; Cruz, L. J.; Ossendorp, F. A.; Jager, M. J. Current challenges and opportunities of photodynamic therapy against cancer. *Pharmaceutics* **2023**, *15*, 330.
2. Chu, J. C. H.; Wong, C. T. T.; Ng, D. K. P. Toward precise antitumoral photodynamic therapy using a dual receptor-mediated bioorthogonal activation approach. *Angew. Chem. Int. Ed.* **2023**, *62*, e202214473.
3. Zhang, J.; Yang, P. L.; Gray, N. S. Targeting cancer with small molecule kinase inhibitors. *Nat. Rev. Cancer* **2009**, *9*, 28-39.

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Time-Resolved XFEL Pump–Probe Analysis Reveals Structural–Electronic Coupling at Metal Sites in Cytochrome *c* Oxidase

Takahiro Watanabe[a], Wakaba Noda[a], Takanori Nakane[b], Tetsuo Katayama[c], Atsuhiro Shimada[d]

[a]*Department of Life Science and Chemistry, Gifu University*
[b]*Institute for Protein Research, Osaka University*
[c]*Japan Synchrotron Radiation Research Institute*
[d]*Faculty of Applied Biological Science, Gifu University*

Bovine cytochrome *c* oxidase (CcO) reduces molecular oxygen (O_2) to two water molecules, coupled with unidirectional proton transfer from the mitochondrial matrix (N-side) to the intermembrane space (P-side). Bovine heart CcO contains four redox-active metal sites (Cu_A, heme *a*, heme a_3, and Cu_B) that are essential for its activity. It has been proposed that each pump proton is transferred from N-side to P-side by harnessing electrostatic interactions between protons and metal sites that are oxidized or reduced upon sequential electron transfer from cytochrome *c* to the O_2 reduction site, composed of heme a_3 and Cu_B, via the low-potential sites Cu_A and heme *a*. Furthermore, for efficient and unidirectional proton transfer, the conformation of the proton pump pathway, the so-called H-pathway, is regulated depending on the electronic states of the metal sites. However, how electronic state changes at individual metal sites are coupled to structural rearrangements along the H-pathway remains incompletely understood.

In this study, to elucidate the coupling between metal-site electronic changes and proton pump pathway rearrangements, we simultaneously collected X-ray emission spectroscopy (XES) data to probe the electronic states of the metal sites and X-ray diffraction (XRD) data to visualize structural changes along the H-pathway. To avoid X-ray-induced reduction damage and to capture early-stage proton pump–related structural changes together with the electronic state changes at the metal sites, we performed serial femtosecond crystallography using CO-bound reduced CcO microcrystals at SACLA, X-ray free electron laser (XFEL) facility. In the presence of O_2, irradiation with 532 nm light (pump laser) induces replacement of CO bound to Fe_{a3} at O_2 reduction site in CcO with O_2 and initiates the catalytic cycle.

At 100 μs after pump laser irradiation, Kα difference spectrum of Fe exhibited a slight shift toward higher energy, whereas no significant changes were detected in the Cu Kα spectrum. These results indicate CO dissociation from the Fe_{a3} without accompanying redox and electron spin state changes at the Cu sites, suggesting that O_2 binding to the O_2 reduction site had not yet occurred within 100 μs after CO release.

Consistently, XRD data revealed decreased ligand-derived electron density at the O_2 reduction site following laser irradiation, supporting CO dissociation. Additionally, structural changes were detected along the H-pathway. Together, these findings indicate that structural dynamics of the proton pump pathway are tightly coupled to electronic state changes at the metal sites in CcO.

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Regulating Cell Death Induced by Photodynamic Therapy with Phthalocyanine through Incorporation on a Zeolitic Imidazolate Framework

Jiaen Xie[a], Meijun Wang[b], Xiaoyan Cui[b], Kwan T. Chow[b]*, Pui-Chi Lo[b]*, and Dennis K. P. Ng[a]*

[a] *Department of Chemistry, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China*
[b] *Department of Biomedical Sciences, City University of Hong Kong, Kowloon, Hong Kong, China*

Photodynamic therapy (PDT) has emerged as a promising treatment modality for cancer [1]. Its efficacy, however, is often limited by the low tumor specificity, the hypoxic tumor microenvironment, and the weak immunogenicity of apoptosis-dominated cell death [2]. With a view to addressing the last issue, we report herein a simple yet efficient nanoplatform constructed by incorporating a zinc(II) phthalocyanine-based photosensitizer (Pc) on the zeolitic imidazolate framework-90 (ZIF-90) via a Schiff base reaction. The resulting nanosystem labeled as Z@Pc exhibited pH and adenosine triphosphate (ATP) responsive properties, enabling targeted release of Pc molecules and Zn^{2+} ions in the acidic tumor microenvironment and ATP-rich subcellular compartments. Under red-light irradiation, Z@Pc generated reactive oxygen species efficiently in cancer cells, causing cell death with a half maximal inhibition concentration of ca. 0.1 μM (with respect to Pc) for 4T1 cells. Interestingly, the cell death pathway induced by Pc was switched from predominately apoptosis to pyroptosis by using ZIF-90 as a nanocarrier. Mechanistic studies revealed that the Zn^{2+} ions released upon decomposition of ZIF-90 played a key role in activating caspase-1/gasdermin D-dependent pyroptosis [3]. This pyroptosis-inducing PDT strategy significantly enhances the anti-tumor efficacy, providing a new paradigm in immuno-PDT against cancer.

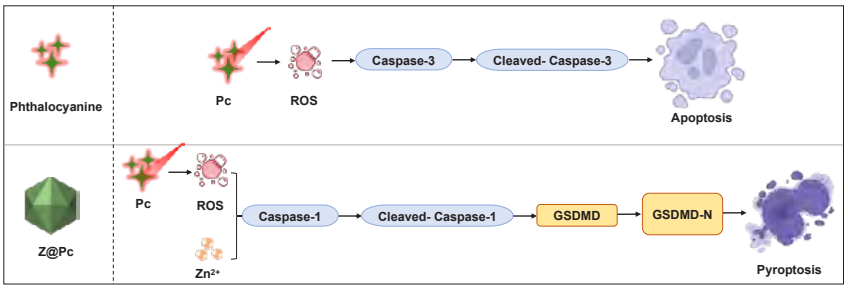


Figure 1. The working principle of Z@Pc switches the death mode from apoptosis to pyroptosis.

This work was supported by a Collaborative Research Fund from the Research Grants Council of the Hong Kong Special Administrative Region, China (ref. no. C4057-24GF).

REFERENCES

1. Dolmans, D. E. J. G. J.; Fukumura, D.; Jain, R. K. Photodynamic therapy for cancer. *Nat. Rev. Cancer* **2003**, *3*, 380−387.
2. Huis in't Veld, R. V.; Heuts, J.; Ma, S.; Cruz, L. J.; Ossendorp, F. A.; Jager, M. J. Current challenges and opportunities of photodynamic therapy against cancer. *Pharmaceutics* **2023**, *15*, 330.
3. Shi, J.; Gao, W.; Shao, F. Pyroptosis: gasdemin-mediated programmed necrotic cell death. *Trends Biomed. Sci.* **2017**, *42*, 245−254.

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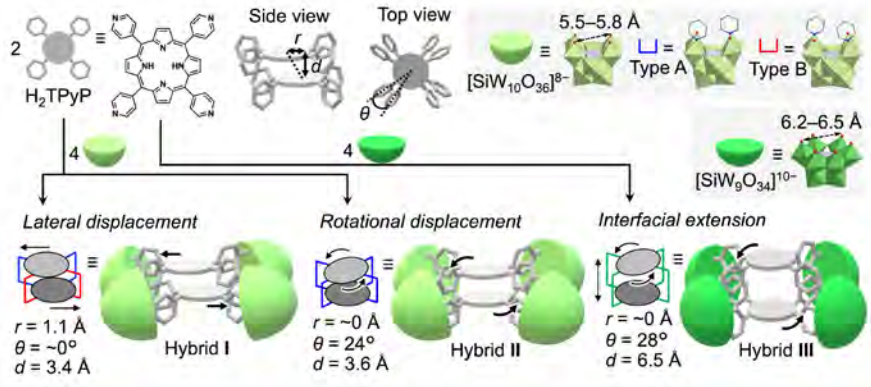
Engineering of Cofacial Porphyrin Dimers Using Polyoxometalates and Their Photocatalysis

Masahiro Yamaguchi,[a] Kaito Shioya,[a] Chifeng Li,[a] Kentaro Yonesato,[a,b] Kei Murata,[c] Kazuyuki Ishii,[d] Kazuya Yamaguchi,[a] Kosuke Suzuki[a,b]

[a]*School of Engineering, The University of Tokyo,* [b]*Graduate School of Frontier Sciences, The University of Tokyo,* [c]*RIKEN Center for Sustainable Resource Science.* [d]*Institute of Industrial Science, The University of Tokyo.*

Porphyrins serve as highly efficient photocatalysts, attributed to their intense visible-light absorption and their capacity to sensitize molecular oxygen ($^3O_2$) to reactive singlet oxygen ($^1O_2$). However, they are easily decomposed by the reaction with the generated $^1O_2$, which limits their long-term applicability. Therefore, the development of porphyrin photocatalysts with both high activity and durability is highly desired. Cofacial porphyrin dimers exhibit unique photophysical and catalytic properties derived from the arrangement of porphyrins.[1] Nevertheless, porphyrin dimers bridged by organic linkers or metal-ion linkers have faced challenges in achieving precise control over their cofacial structures.

Herein, we presented a novel strategy for fine-tuning the structures of cofacial porphyrin dimers by employing lacunary polyoxometalates (POMs) as linkers, thereby enhancing both their photocatalytic activity and durability.[2,3] The diverse coordination modes and structural versatility of lacunary POMs enable fine-tuning of porphyrin displacement and inter-porphyrin distances. In addition, the heavy-atom effect of the POMs promotes efficient $^1O_2$ generation, while the rigid cofacial stacking induced by POM coordination provides exceptional durability against $^1O_2$. Hybrid **I**, formed through self-assembly of two 5,10,15,20-tetra(4-pyridyl)porphyrin molecules and four divacant $[SiW_{10}O_{36}]^{8-}$ units, exhibited a laterally displaced structure (1.1 Å) with an interfacial distance of 3.4 Å. In contrast, hybrid **II**, obtained using the same POM but with a different coordination mode, exhibited rotational displacement but no lateral displacement, and a longer interfacial distance (3.6 Å). Replacing $[SiW_{10}O_{36}]^{8-}$ with trivacant $[SiW_9O_{34}]^{10-}$ yielded hybrid **III**, which featured an extended interfacial distance (6.5 Å) and greater rotation. Furthermore, hybrids **I** and **II** exhibited superior photocatalytic activity in the aerobic oxidation of organic substrates compared to free porphyrins. This enhancement is attributed to the high $^1O_2$ generation efficiency, likely due to the heavy-atom effect of POMs, and to the exceptional durability against $^1O_2$ achieved through the structural rigidity of the POM-based cofacial porphyrin dimers.



REFERENCES

1. A. Satake, Y. Kobuke, *Org. Biomol. Chem.* **2007**, *5*, 1679.
2. M. Yamaguchi, K. Shioya, C. Li, K. Yonesato, K. Murata, K. Ishii, K. Yamaguchi, K. Suzuki, *J. Am. Chem. Soc.* **2024**, *146*, 4549.
3. M. Yamaguchi, K. Yonesato, K. Shioya, C. Li, K. Murata, K. Ishii, K. Yamaguchi, K. Suzuki, *Chem. Sci.* **2025**, *16*, 9178.

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Bimetallic porphyrin PET radiotracers for Low-Dose MRI contrast enhancement

Yik-Hoi Yeung[a], Pak-Lun Lam[a], Chen Xie[a], Ho-Fai Chau[a], Nicholas J. Long[c], Ga-Lai Law[a], and Ka-Leung Wong[a,b]

[a] *Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Hong Kong SAR, klgwong@polyu.edu.hk*
[b] *Department of Chemistry, The City University of Hong Kong, Kowloon, Hong Kong SAR, klwong@cityu.edu.hk*
[c] *Department of Chemistry, Imperial College London, White City Campus, London W12 0BZ, United Kingdom, n.long@imperial.ac.uk*

In medical imaging, concerns about the risks associated with imaging agents have been consistently raised by doctors and patients, and ongoing efforts are underway to cautiously explore safer, more efficient compounds. There is a continued interest in combining the well-known imaging modalities of positron emission tomography (PET) and magnetic resonance imaging (MRI). However, no single-molecule probe has been reported to offer dual-modal imaging without performance degradation. We herein present a potential solution in which the compound PGaLGd incorporates radioactive Ga(III) for PET imaging whilst simultaneously exhibiting MRI contrast through a coordinated Gd(III) ion, albeit at low concentrations/doses. In addition to elucidating MRI-enhancing mechanisms using computational chemistry techniques, our compound has been shown to be a successful dual-imaging agent for both PET and MRI in mice. Additionally, we conducted comprehensive *in vitro* and *in vivo* studies to assess biosafety and photodynamic therapeutic potential across various cell lines and organoids. We have placed importance on interlinking structures, coordinated metals, adjacent ligands, and frontier molecular orbitals in our probe design to enhance water relaxation ability and move towards the design of next-generation low-dose imaging agents.

REFERENCES

1. C. Xie, X. Li, L. Zhang, H.-F. Chau, W. Thor, W. S. Tam, B. Woolley, M. Jiang, C.-F. Ng, M. Botta, T. Zhang, N. J. Long, G.-L. Law, K.-L. Wong, *Chem. Eng. J.* **2024**, 495, 153350

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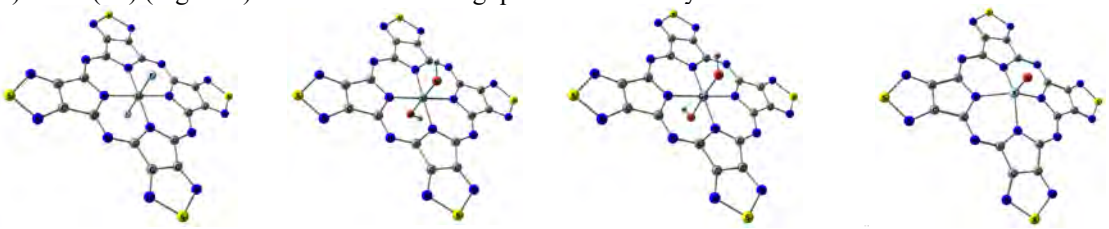
Molecular structure and electron density distribution of tetrakis(1,2,5-thiadiazole)porphyrazine complexes

Dmitriy A. Vyalkin, Ulyana A. Petrova, Alina A. Knyazeva, Alexey V. Eroshin, Yuriy A. Zhabanov

Ivanovo State University of Chemistry and Technology, Research Institute of Chemistry of Macroheterocyclic Compounds, 153000 Ivanovo, Russia

Tetraazaporphyrins are macrocyclic analogs of porphyrins, containing the nitrogen atoms instead of meso-carbon atoms. Tetrakis(1,2,5-thiadiazole)porphyrazine (TTDPz) and their metal complexes are of special interest, due to the macrocyclic compounds involved in viable processes such as photosynthesis, cellular respiration, etc.

In this work the study of molecules of tetrakis(1,2,5-thiadiazole)porphyrazine with Si(IV), Ge(IV), Ti(IV) and V(IV) (Figure 1) was carried out using quantum chemistry calculations.



SiF_2TTDPz $Si(OH)_2TTDPz$ $Ge(OH)_2TTDPz$ TiOTTDPz and VOTTDPz

Figure 1. Molecular structures of tetrakis(1,2,5-thiadiazole)porphyrazine complexes with Si(IV), Ge(IV), Ti(IV) and V(IV).

The optimization of the structural parameters of the considered complexes was carried out using DFT approach, PBE0-D3/def2-TZVP taking into account Grimme's dispersion correction. Theoretical electronic absorption spectra were obtained using the TDDFT method. The number of excited states was 100. Electron density distribution analysis was performed within the "Atoms in Molecules" theory QTAIM using MultiWFN software package. Molecular structures were visualized by ChemCraft program.

It has been established that the optical properties of TTDPz complexes may be regulated by three main factors: the nature of the central metal atom (particularly, its mass and electron configuration), oxidation state, and the nature of the axial ligands.

An analysis of the electron density distribution shows that replacing the central atom (Si or Ge) or axial ligands (F or OH) has a minor effect on the electron density distribution in the peripheral rings. Replacing fluorine with a hydroxyl group in **SiX_2TTDPz** reduces the ionic contribution of the Si–X (X=F, OH) bond and increases its covalent component. Compared to **SiX_2TTDPz**s, the **$Ge(OH)_2$TTDPz** complex exhibits the highest delocalization indices for the M–X (X=F, OH) bond, indicating more efficient covalent overlap of germanium orbitals with pi orbitals of axial ligands. Considering **TiOTTDPz** and **VOTTDPz**, it can be noted that the properties of the porphyrazine core are independent of the metal type, because the influence of the central atom is limited by a macrocyclic cavity and does not reach the peripheral thio groups. The high ellipticity of the N_t–S bonds confirms the active participation of sulfur atoms in the general π-conjugation system in both **TiOTTDPz** and **VOTTDPz** compounds.

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