

4^{eme} Journée de Chimie Supramoléculaire



JCS-2026 Marseille

May 28-29



Program and book of abstracts

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Organizing committee

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Program

Thursday, May 28, 2026

11h30	Opening of registration, poster installation Lunchbox distribution and coffee break			
13h30	JCS-2026 opening, Welcome works			
13h50	Chair : D. Frath	Lecture 1	Mihail BARBOIU Prix André Collet <i>Artificial Water Channels toward Biomimetic Membranes for Desalination</i>	
14h30		CO-1	Arnaud TILLET <i>From molecular complexes to giant ordered architectures: supramolecular polymerization of [B₁₂I₁₂]²⁻/γ-cyclodextrin into helical nanotubes and hexagonally ordered networks</i>	
14h45		CO-2	Diana DEAI BESS <i>Supramolecular Helical Polymers for Bifunctional Asymmetric Organocatalysis</i>	
15h00		Flash Comm 1-6		FC-01. Beatris Onzimba <i>Caged Macrocycles: Towards non-heme bioinspired catalysts</i>
				FC-02. Yanis Tigherghar <i>Metal complexes based on modified cyclodextrins for the development of catalytic reactions in cells</i>
	FC-03. Elsa Maarek <i>Elaboration of non fullerene acceptors for Indoor Photovoltaics</i>			
	FC-04. Louise Pfeiffer <i>Porphyrin cages for photoredox catalysis of heterobiaryls</i>			
	FC-05. Dania Daou <i>Not going back: Unidirectional movement by intramolecular one-way ratcheting of functionalized cyclodextrin</i>			
	FC-06. Pierre-Antoine Dupin <i>Low-Symmetry Hemicyptophanes functionalized with Azaphosphatrane derivatives</i>			
15h30	Coffee break and Poster session			

16h00		Lecture 2	Mickaele HARDIE <i>Supramolecular cages and network assemblies from pyramidal host-ligands</i>
16h40		CO-3	Loïc PINTO <i>Novel anionic phosphine-based supramolecular cages</i>
16h55		CO-4	Louise MITON <i>Hierarchical Sequence Control Enables Assembly of a Triple Helix with Preferred Handedness</i>
17h10	Chair : B. Chatelet	Flash Comm 7-12	FC-07. Chloé Jamalkhan <i>Ordered Honeycomb Host–Guest Networks on HOPG for Supported Asymmetric Catalysis</i> FC-08. Axel Eisenbeth <i>Chiroptical bis-(acridinium-Zn(II)porphyrin) Tweezers</i> FC-09. Jaya Preethi Jayaprakasam <i>Möbius hexaphyrins with an overhanging metal binding site as unprecedented allosteric receptors</i> FC-10. Lucrezia Trevisan <i>Insights into self-assembly mechanisms and electrical properties of tetrazinebased supramolecular polymers</i> FC-11. Yohan Zarate <i>Mechanical disruption of β-Amyloid fiber analogs by out-of-equilibrium operation of light-driven molecular motors</i> FC-12. David Leparfait <i>Design, Synthesis and Physicochemical Properties of Nitrogen Modified Cryptophane A</i>
17h40	Cocktail and Poster session		
19h45	End		

8h30	Chair : S. Durot	Lecture 3	Hennie VALKENIER <i>Supramolecular Ion Receptors for Transmembrane Transport</i>
9h10		CO-5	Hugo LAIGLE <i>Imidazole-Semicarbazones as Photo-Controllable Ion and Water Transporters</i>
9h25		CO-6	Thanaphon KHRUEAWATTHAWET <i>Möbius hexaphyrin with a metallo-allosteric site: interplaying a coordinating arm and coordinating strap</i>
9h40		CO-7	Benjamin MOUROT <i>Regioisomerism-Dependent Optoelectronic and Supramolecular Behaviour of BisAzaCoroneneDiimide N-oxides</i>
9h55		Flash Comm	Société Advion Interchim Société Merck JCS-2026 participants picture ! 
10h10	Coffee break and Poster session		
10h40	Chair : S. Goeb	CO-8	Vivien ANDRIEUX prix thèse SCF-Supra <i>Electron-Responsive Conductive Supramolecular Materials Based on Viologens Self-Assembly</i>
10h55		CO-9	Simon PASCAL <i>Azacalixarene's Midlife Crisis: Cyanide Capture and Spontaneous Liberation</i>
11h10		CO-10	Mickaël MENAND <i>pH-Gated Transient Supramolecular Polymerization of Cyclodextrins</i>
11h25		CO-11	Noémie LALAOUI <i>Supramolecular Confinement Enables Selective CO₂-to-CO Conversion in Water</i>
11h40		CO-12	Jean-François LONGEVIAL <i>Self-Assembled Organometallic Cages from poly-NHC Perylenebisimide Based Ligands</i>
11h55	Lecture 4	Nicolas GIUSEPPONE Prix Henri Le Chatelier <i>Using artificial molecular motors to drive complex chemical systems out-of-equilibrium</i>	
12h35	Awards Ceremony, Closing remarks		

Lectures



Lecture 1

Dr. Mihail Barboiu

Institut Européen des Membranes, Université Montpellier

Prix André Collet



Mihail Barboiu received his PhD in 1998 from University of Montpellier. He is DR1 CNRS Research Leader at the Institut Européen des Membranes in Montpellier. A major focus of his research is Dynamic Constitutional Chemistry toward adaptive biomimetic membranes. Dr Barboiu has received in 2004, the EURYI Award in Chemistry and in 2015, the RSC Surfaces and Interfaces Award and Prix André Collet 2024, Groupe de Chimie Supramoléculaire, DCO, Société Chimique de France for the development of Artificial water channels. Artificial Water Channels may be most innovative new idea for water purification membranes and aqueous separations.

<http://rsc.li/water-channels>

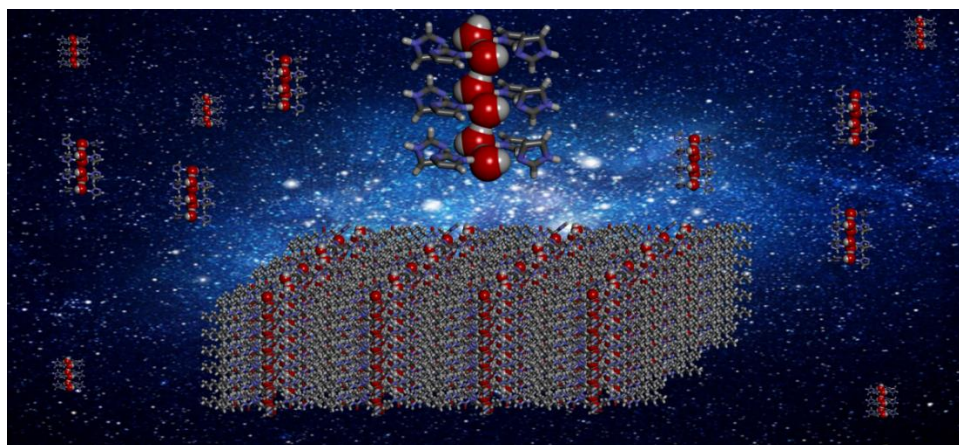
<https://iem.umontpellier.fr/en/mihail-barboiu/>

Artificial Water Channels toward Biomimetic Membranes for Desalination

Mihail Barboiu

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Aquaporins (AQPs) are natural proteins able to selectively transport water across cell membranes. Heterogeneous H-bonding of water with inner wall of the pores of AQPs is of maximal importance regarding the optimal stabilization of water clusters within channels leading to selective water transport against ions. To get deeper insight into the water permeation mechanisms, simpler artificial water channels (AWCs) have been developed. Several H-bonding motifs (i.e. imidazole, polyhydroxy, etc.) have been reported as distinct and efficient for water-cluster stabilization within AWCs. Herein we describe several membrane pore configurations able to stabilize, like in AQPs water molecules *via* different H-bonding groups. The crystal structures reveal that stable water superstructures are formed in the solid state, accommodating water clusters or water-wires. Molecular simulation confirmed that AWC-channels can generate stable supramolecular porous sponges, featuring multivalent water H-bonding units that serve as water-cluster relays within the channel. To the best of our knowledge, this works are a rare biomimetic example of the importance of water-cluster stabilization *via* multivalent H-bonding and toward selective transport through water channels and further translated for the fabrication of efficient biomimetic membranes for desalination .



1. I.-M. Andrei, W. Chen, M. Baaden, S. Vincent, M. Barboiu, *J. Am. Chem. Soc.*, **2023**, *145*, *40*, 21904–21914
2. I. -M. Andrei, Iuliana; A. Chaix, B.T. Benkhaled, R. Dupuis, C. Gomri, E. Petit, Eddy, M. Polentarutti, A. van der Lee, Arie, M Semsarilar, M. Barboiu *J. Am. Chem. Soc.*, **2023**, *145*, 21213–21221.
3. L.-B. Huang, F. Mamiya, M. Baaden, E. Yashima, M. Barboiu, *ACS Appl. Mater. Interfaces* **2023**, *15* 40133.
4. I.-M. Andrei, D. Strilets, S. Fa, M. Baaden, T. Ogoshi, M. Barboiu, *Angew. Chem. Int. Ed.* **2023**, e202310812
5. D.-D. Su, S. Ulrich, M. Barboiu, *Angew. Chem. Int. Ed.* **2023**, *62*, e202306265
6. M. Di Vincenzo, A. Tiraferri, V.-E. Musteata, S. Chisca, R.Sougrat, L.-B. Huang, S. P. Nunes, M. Barboiu, *Nature Nanotechnol.* **2021**, *16*, 190-196.
7. D. Strilets, S. Fa, A. Hardiagon, M. Baaden T. Ogoshi, M. Barboiu, *Angew. Chem. Int. Ed.* **2020**, *59*, 23213.
8. S.-P. Zheng, J.-J. Jiang, A. van der Lee, M. Barboiu *Angew. Chem. Int. Ed.* **2020**, *59*, 18920-18296.
9. M. Di Vincenzo, et al. *Proc. Natl. Acad. Sci. USA*, **2021**, *118*(37), e2022200118.
10. L.-B. Huang, M. Di Vincenzo, M. Göktuğ Ahunbay, A. van der Lee, D. Cot, S. Cerneaux, G. Maurin, and M. Barboiu, *J. Am. Chem. Soc.* **2021**, *143*, 14386-14393.

Lecture 2

Pr. Michaele Hardie

Faculty of Engineering and Physical Sciences, University of Leeds, UK

Invited speaker



Pr. Michaele Hardie : "I did my undergraduate degree and PhD at the University of Melbourne in Australia. My PhD (1996) was on the synthesis and X-ray structure determination of coordination polymers working under the supervision of Richard Robson and Bernard Hoskins. I did post-doctoral work at Melbourne, University of Toledo USA and Monash University, Australia before being appointed lecturer in inorganic chemistry at the University of Leeds in 2001, where I am currently Professor of Supramolecular Chemistry. I was awarded the Royal Society of Chemistry Corday-Morgan Prize in 2011 for most meritorious contributions to chemistry (40 yo or under). I have recently held a visiting professorship at Osaka University (2017). My current research interests are in the area of metallo-supramolecular chemistry and we are particularly interested in the self-assembly of discrete nano-scale metallo-supramolecular cages, and in coordination polymers. Discrete cages often have polyhedral or prismatic structures and tend to feature significant internal space. Hence such assemblies may have potential applications as nano-scale reaction vessels. Coordination polymers are crystalline metal-ligand systems with infinite structures such as chains, helices, grids and 3D lattices. MOFs are a class of coordination polymers with 3D framework structures that are robust and porous. These materials may be useful for a number of applications, including molecular separations, catalysis and molecular storage."

<https://eps.leeds.ac.uk/chemistry/staff/4189/professor-michaele-hardie>

Supramolecular cages and network assemblies from pyramidal host-ligands

James J. Henkelis, Samuel Oldknow, Victoria E. Pritchard, Matthew P. Snelgrove, Flora Thorp-Greenwood, Michaele J. Hardie.

School of Chemistry, University of Leeds, Leeds, UK

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Cyclotrimeratrylene (= CTV) is a pyramidal host molecule that can be functionalised to form tripodal or hexapodal cavitand L ligands. These can be used to form multi-metallic assemblies including discrete metallated complexes, coordination cages¹ and coordination polymers² and other networked materials.³ Examples of metallo-cages include trigonal bipyramidal M_3L_2 cages, M_6L_8 stella octangula cages and $M_{12}L_8$ cubes. Cages and other assemblies may show topological complexity, and functionality such as luminescence and/or whole-cage photoisomerisation can be embedded in the cages. A variety of coordination polymers can also be formed and these often show host-guest interactions both within networks and between networks. Formation of networks of cages prevents such host-guest interactions and allows materials with hierarchical pore spaces to be synthesised. These have shown guest-uptake or photocatalytic activity and clusters of cage-catenanes undergo solid-state structural transformations on solvent-exchange.³

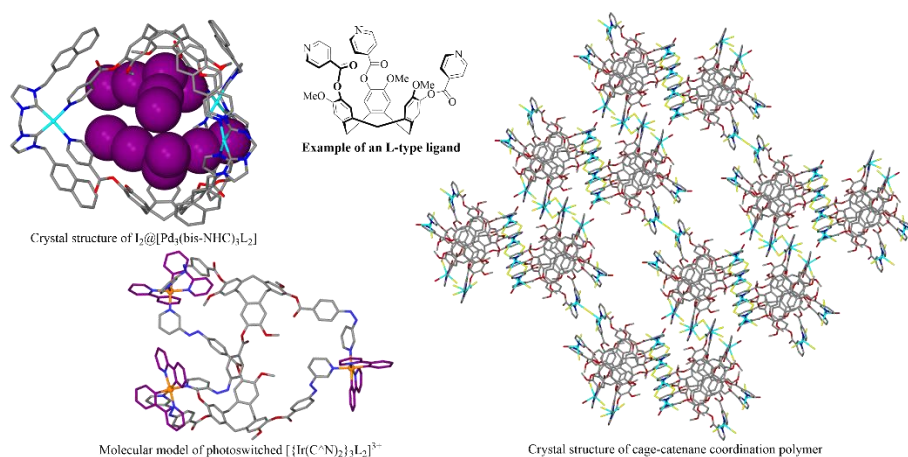


Figure 1. Assemblies of pyramidal host-ligands L; I_2 -capture by Pd_3L_2 cage; photo-switched Ir_3L_2 cage; and Cu-Cl bridged cage-catenanes.

Acknowledgements. University of Leeds, Leverhulme Trust, EPSRC and Diamond Light Source are acknowledged for support.

¹ S. Oldknow, D. Rota Martir, V. E. Pritchard, M. A. Blitz, C. W. G. Fishwick, E. Zysman-Colman, M. J. Hardie, M. J. *Chem. Sci.* **2018**, *9*, 8150; J. J. Henkelis, C. J. Carruthers, S. E. Chambers, R. Clowes, A. I. Cooper, J. Fisher, M. J. Hardie, *J. Am. Chem. Soc.* **2014**, *136*, 14393

² M. P. Snelgrove and M. J. Hardie, *CrystEngComm*, **2021**, *23*, 4087

³ F. L. Thorp-Greenwood, A. N. Kulak, M. J. Hardie, *Nature Chemistry*, **2015**, *7*, 526

⁴ M. P. Snelgrove, N. N. Sergeeva, M. J. Hardie, *Chem. Eur. J.* **2025**, *31*, e202403692

Lecture 3

Dr Hennie Valkenier-van Dijk

Engineering of Molecular NanoSystems, Université Libre de Bruxelles, Be

Invited speaker



Hennie Valkenier studied Chemistry at the University of Groningen (NL) and obtained her PhD from this university in 2011 with a thesis on Molecular Electronics. After a year of teaching in West-Africa, she joined the group of Tony Davis at the University of Bristol as a postdoc to develop transmembrane transporters for chloride. In 2015, she moved to the Engineering of Molecular NanoSystems laboratory at the Université libre de Bruxelles, where she worked for a year on the functionalisation of gold nanoparticles, before returning to transmembrane transport research funded by an FNRS fellowship. In 2018, she has obtained a permanent position as FNRS Research Associate at the Université libre de Bruxelles and was awarded an ERC starting grant to develop new classes of anion transporters. Since 2025 she is also an investigator of the WEL Research Institute.

<https://emns.polytech.ulb.be/en/team/hennie-valkenier>

Supramolecular Ion Receptors for Transmembrane Transport

Hennie Valkenier ^[a,b]

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Synthetic ion receptors bind anions reversibly and can be used for the transport of anions across lipid bilayers, which form a barrier for the free diffusion of ions and other hydrophilic species. Such synthetic anion transporters can find applications in biology, for instance by disruption of homeostasis leading to toxicity, as is relevant for anticancer and antimicrobial applications. We develop transporters for different ions as well as the methods to study the transport process in liposomes.

Whereas most of the research on anion transport focusses on chloride, we have overcome a series of challenges¹ to develop the first synthetic transporter for inorganic phosphate, featuring a strapped calix[4]pyrrole.^{2,3}

Secondly, we have developed calix[4]arene-based Cu⁺ ionophores⁴ and have studied the Cu⁺ transport into liposomes and yeast cells. Furthermore, these ionophore have a highly potent anti-cancer activity on hepatocytes and synchrotron X-ray fluorescence experiments allowed to attributed this toxicity to a redistribution on intracellular copper pools.⁵

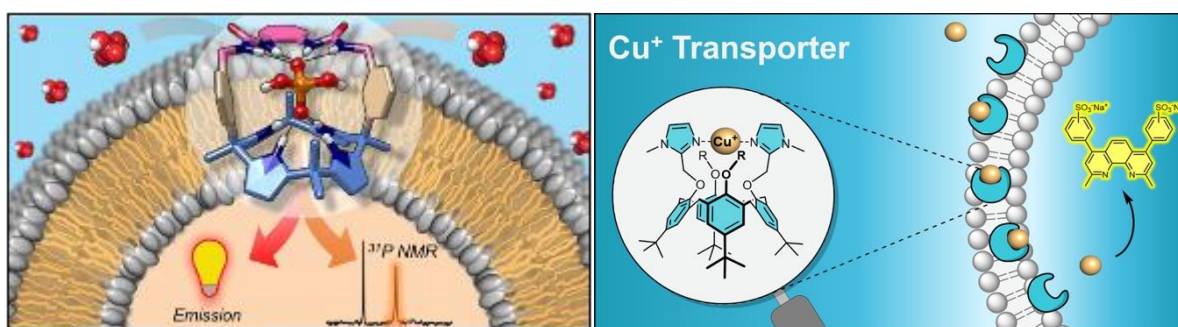


Figure 1. A strapped calix[4]pyrrole and transporter for H₂PO₄²⁻ (left) and a calix[4]arene-based Cu⁺ transporter (right).

Acknowledgements. This project has received funding from the European Research Council (ERC, Grant agreement No. 802727) and the Fonds de la Recherche Scientifique – FNRS for Research Project T.0227.23. H.V. is a Research Associate of the Fonds de la Recherche Scientifique – FNRS and a WEL Research Institute investigator and thanks COST Action CA22131, LUCES–Supramolecular Luminescent Chemosensors for Environmental Security, supported by COST (European Cooperation in Science and Technology).

¹ K. Norvaisa, A. Torres-Huerta and H. Valkenier, *Curr. Opin. Chem. Biol.*, **2024**, *83*, 102542.

² A. Cataldo, K. Norvaisa, L. Halgreen, S. E. Bodman, K. Bartik, S. J. Butler, H. Valkenier, *J. Am. Chem. Soc.* **2023**, *145*, 16310.

³ A. Torres-Huerta, K. Norvaisa, A. Cataldo, P.-O. Tits, P. R. Panda, C. M. Dias, A. P. Davis, S. E. Bodman, S. J. Butler, H. Valkenier, *ChemistryEurope* **2025**, *3*, e202400076.

⁴ N. Renier, O. Reinaud, I. Jabin, H. Valkenier, *Chem. Commun.* **2020**, *56*, 8206–8209.

⁵ N. Renier, G. Weyckmans Mele, P. Lelièvre, M. Boeckstaens, R. Lavendomme, A. Aydogan, Y. Dussein, P. Charbonnier, L. Puillet Anselme, B. Chovelon, H. Castillo-Michel, N. Tumanov, J. Wouters, L. Sancey, B. Busser, A. M. Marini, G. Veronesi, I. Jabin, A. Deniaud, H. Valkenier, *J. Am. Chem. Soc.* **2026**, *148*, 593.

Lecture 4

Pr. Nicolas Giuseppone

Institut Charles Sadron, Univ. Strasbourg

Prix Henry Le Chatelier



Nicolas Giuseppone obtained his PhD in asymmetric catalysis (Prof. H.B. Kagan's laboratory, Paris-Saclay), completed a postdoctoral fellowship in total synthesis (Prof. K.C. Nicolaou's laboratory, Scripps Research, San Diego), and subsequently moved into the field of supramolecular chemistry as a CNRS Research Fellow in Prof. J.-M. Lehn's laboratory in Strasbourg.

In 2008, he established his own research group and was promoted to Exceptional Class Professor in 2016. He served as Deputy Director of the Institut Charles Sadron (2012–2023) and Director of the Grand Est Federation for Materials and Nanoscience Research (2018–2023). His research focuses on supramolecular chemistry, molecular machines, and functional materials.

In 2024, he was awarded the CNRS Silver Medal in recognition of the originality, quality, and significance of his research contributions.

<http://sams.ics-cnrs.unistra.fr/membres/membres-actuels/membres-permanents/nicolas-giuseppone/>

Using artificial molecular motors to drive complex chemical systems out-of-equilibrium

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Inspired by the protein machinery found in biological systems, and based on the theoretical understanding of the physics of motion at nanoscale, organic chemists have developed a number of molecules that can actuate when triggered by various external chemical or physical stimuli. In particular, basic molecular switches that commute between (meta)stable states, and more advanced molecular motors that produce unidirectional cyclic motions, have been reported. However, the integration of individual molecular motors in a continuous out-of-equilibrium mechanical process that can produce mechanical work at various length scales and up to the macroscale remains an important area to explore.^[1,2] We will discuss advances developed by our group on the collective actuation of artificial molecular motors, which involve their mechanical coupling with polymer and supramolecular self-assemblies. We will show how it becomes possible to integrate them and to make use of their autonomous mechanical work to drive endoenergetic processes in complex systems and active materials.

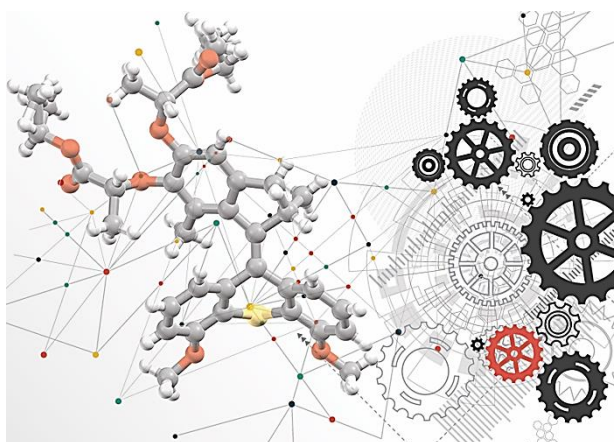


Figure 1. Motor System.

References

- [1] D. Dattler, G. Fuks, J. Heiser, E. Moulin, A. Perrot, Y. Xuyang, N. Giuseppone, *Chem. Rev.* **2020**, *120*, 310-443.
[2] E. Moulin, L. Faour, C. Carmona-Vargas, N. Giuseppone, *Adv. Mat.* **2020**, 201906036.

Oral communications



From molecular complexes to giant ordered architectures: supramolecular polymerization of $[B_{12}I_{12}]^{2-}/\gamma$ -cyclodextrin into helical nanotubes and hexagonally ordered networks

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Nano-ions such as dodecaborate anions exhibit low volumetric charge density, imparting remarkable supramolecular properties through chaotropic effects in aqueous solutions.¹ This powerful solvent effect enables self-assembly with non-ionic organic substances.²

The exceptional ability of $[B_{12}I_{12}]^{2-}$ to bind γ -cyclodextrin simultaneously on both faces, enabled by the chaotropic effect and good size-matching, drives supramolecular polymerization from 2D sheet-like intermediates to monodisperse helical nanotubes that assemble into hexagonally ordered networks.

We investigate this hierarchical self-assembly using multi-scale characterization. ¹H NMR spectroscopy probes the dual-face inclusion complexation of $[B_{12}I_{12}]^{2-}$ with γ -cyclodextrin. Small-angle X-ray scattering (SAXS) monitors the progressive increase in structural order from lamellar sheets through cylindrical nanotubes to hexagonal packing. Cryogenic transmission electron microscopy (cryo-TEM) visualizes sheet-like intermediates, monodisperse nanotubes, and their hexagonal arrangement.

This work demonstrates how the chaotropic effect can allow discrete nano-ions to form supramolecular architectures with controlled hierarchical organization.

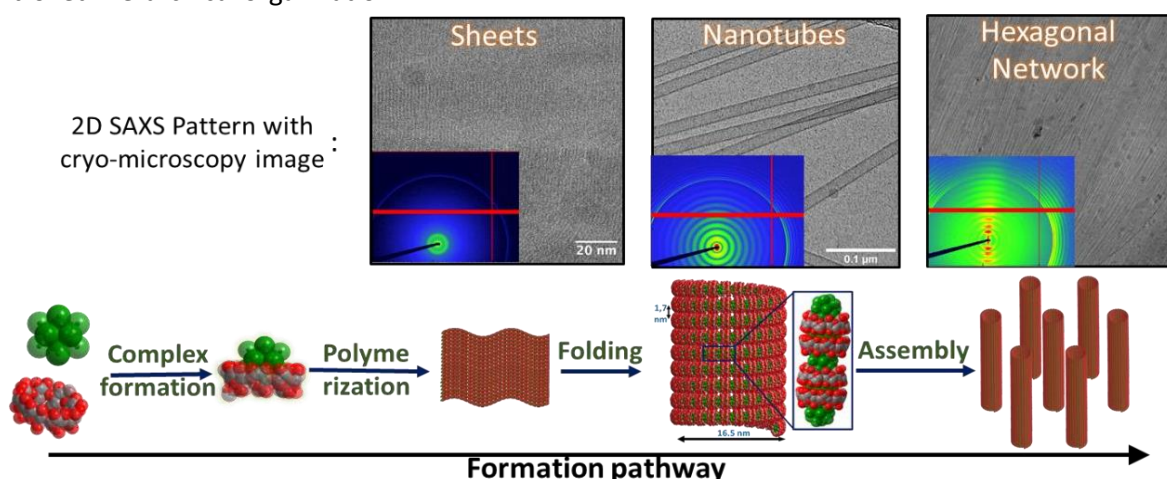


Figure 1 : At the bottom: representation of the formation pathway from discrete species to sheets, nanotubes and hexagonal network. At the top: Cryogenic electron microscopy images with their 2D saxs pattern

[1] Assaf, K. I.; Nau, W. M. *Angew. Chem. Int. Ed.* **2018**, 57 (43), 13968–13981.

[2] (a) Yao, S.; Falaise, C.; Ivanov, A. A.; Leclerc, N.; Hohenschutz, M.; Haouas, M.; Landy, D.; Shestopalov, M. A.; Bauduin, P.; Cadot, E., *Inorg. Chem. Front.* **2021**, 8 (1), 12–25. (b) Khelifi, S.; Marrot, J.; Haouas, M.; Shepard, W. E.; Falaise, C.; Cadot, E. *J. Am. Chem. Soc.* **2022**, 144 (10), 4469–4477. (c) Naskar, B.; Diat, O.; Nardello-Rataj, V.; Bauduin, P. *J. Phys. Chem. C* **2015**, 119 (36), 20985–20992.

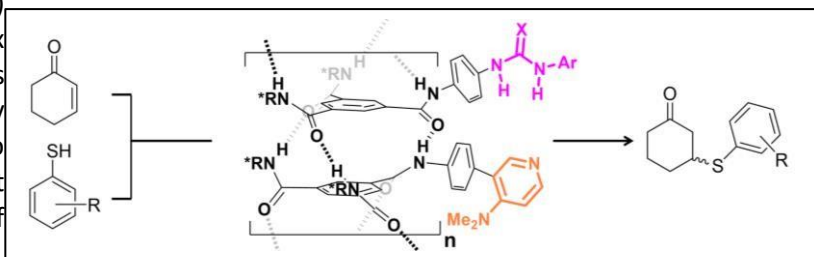
Supramolecular Helical Polymers for Bifunctional Asymmetric Organocatalysis

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The development of asymmetric organocatalytic transformations has highlighted the power of cooperative activation strategies for promoting enantioselective carbon–heteroatom bond formation under mild conditions.¹ Most organocatalysts rely on the interplay between complementary catalytic sites to simultaneously enhance reactivity and stereocontrol; however, these catalysts lack modularity and adaptability due to their covalent nature. Our group demonstrated that intrinsically achiral catalytically active groups located at the periphery of supramolecular helices composed of benzene-1,3,5-tricarboxamide monomers experience the chiral environment of the helices and promote Rh- and Cu-mediated reactions in a highly enantioselective manner.² These catalysts display unique properties: they are modular, operate with a minimal amount of chirality inducers^{2b} and can be switched in real time in order to perform stereodivergent catalysis.^{2d} Built on this framework, we now report the design of BTA assemblies combining two distinct chiral monomers, enabling precise spatial organization of functional groups at the periphery of the dynamic helices. Investigation of the conjugate addition of thiols to enone reveals the bifunctional mode of action of the supramolecular catalyst, wherein basic and hydrogen-bonding sites act synergistically to activate the thiol and the enone, respectively. Advantages of our approach relatively to conventional organocatalysts will be particularly emphasized: i) enantiodivergent behavior achieved by adjusting the ratio of the monomers thanks to chirality induction through the pseudo majority-rule effect, ii) access to a library of bifunctional catalysts ($n \times n$) starting from n monofunctional catalysts thus allowing rapid catalyst optimization, iii) highly tunable catalysis reflected by the possibility to achieve good enantioselectivity in distinct reactions which usually rely on different types of organocatalysts.³



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¹ J. Wang, B. L. Feringa, *Science*, **2011**, *331*, 1429.

² (a) A. Desmarchelier, X. Caumes, M. Raynal, A. Vidal-Ferran, P. W. N. M. van Leeuwen, L. Bouteiller, *J. Am. Chem. Soc.*, **2016**, *138*, 4908. (b) Y. Li, A. Hammoud, L. Bouteiller, M. Raynal, *J. Am. Chem. Soc.*, **2020**, *142*, 5676. (c) M. A. Martínez-Aguirre, Y. Li, N. Vanthuyne, L. Bouteiller, M. Raynal, *Angew. Chem. Int. Ed.*, **2021**, *60*, 4183. (d) R. Chen, A. Hammoud, P. Aoun, M. A. Martínez-Aguirre, N. Vanthuyne, R. Maruchenko, P. Brocorens, L. Bouteiller, M. Raynal, *Nature Commun.*, **2024**, *15*, 4116. (e)

H. Kong, A. Valverde-González, R. Maruchenko, L. Bouteiller, M. Raynal, *Angew. Chem. Int. Ed.*, **2025**, *64*, e202421991. (f) H. Kong, et al.; *Angew. Chem. Int. Ed.*, **2026**, *65*, e21365.

³ D. Deaibess, A. Valverde-González, N. Picois, J. Terlau, M. C. Borralló, L. Bouteiller, V. Mouriès-Mansuy, M. Raynal, *submitted*.

Novel anionic phosphine-based supramolecular cages

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Recently, sterically hindered phosphines have attracted increasing attention in gold chemistry, showing interesting properties in π -activation catalysis (Figure 1a).^{1,2} On the other hand, anionic supramolecular cages have proven efficient in generating reactive (cationic) gold complexes, through electrostatic interactions, and the effect of confinement has been substantiated in a few gold-catalyzed transformations (Figure 1c).^{3,4} While these cages exert a more pronounced steric control than hindered phosphines, partial encapsulation – arising from relatively weak electrostatic interactions – may result in undesired background reactivity occurring outside the cage.

In this context, our project aims at combining these two strategies by developing a new class of standalone anionic phosphine cages (Figure 1b). The central design element is the (tris-catecholate) metal vertex widely used as building block in anionic cages (Figure 1d). Its C_3 symmetry not only complements that of the C_3 symmetric phosphines, but it also offers 3- negative charge, that is essential to cationize gold(I) complexes and achieve catalytic activity. In addition to the well-documented confinement effect, we plan to take advantage of the inherent chirality of the metal vertex (octahedral complex) that is ideally positioned adjacent to the coordination site. Through this integrated approach, we wish to address concrete synthetic challenges (reduced scope in gold catalyzed cyclizations, low stereochemical induction in enantioselective gold(I) catalysis), neither of which can be achieved with hindered phosphines or anionic cages alone.

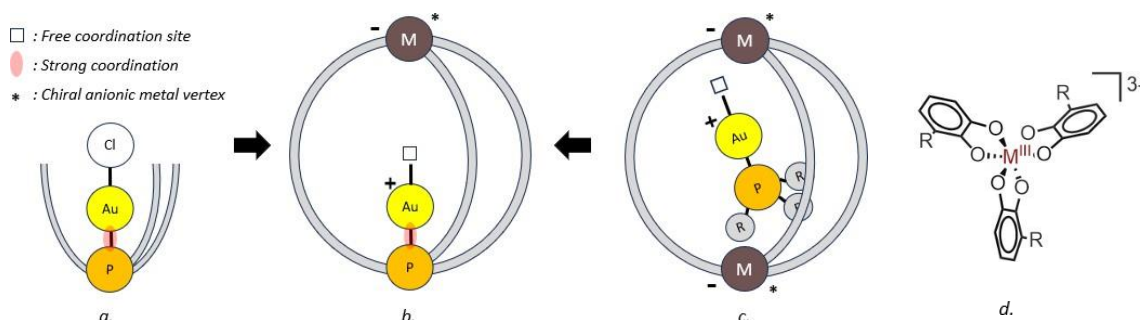


Figure 1. a. Hindered phosphine, b. Hybrid model targeted in this project, c. Anionic supramolecular cage, d. Anionic, chiral metal vertex.

Acknowledgements. Denis Lesage (Sorbonne Université) and Gregori Ujaque (Universitat Autònoma de Barcelona) are acknowledged for their contributions as well as the CNRS and Université de Toulouse for financial support. This project has received funding from the ANR JCJC (CONFICAT)

¹ K. Muratov, F. Gagosz, *Angew. Chem. Int. Ed.* **2022**, *61*, e202203452.

² M. Navarro, M. Holzapfel, J. Campos, *ChemPlusChem* **2023**, *88*, e202300231.

³ Z. J. Wang, C. J. Brown, R. G. Bergman, K. N. Raymond, F. D. Toste, *J. Am. Chem. Soc.* **2011**, *133*, 7358.

⁴ Y. Diack, S. Mallet-Ladeira, D. Lesage, J. S. V. Guerra, D. Bourissou, G. Szalóki, *Chem. Commun.* **2025**, *61*, 8003

Hierarchical Sequence Control Enables Assembly of a Triple Helix with Preferred Handedness

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In nature, the primary sequence of proteins is reliably translated into three-dimensional structures *via* folding. The remarkable fidelity of this process enables them to access levels of functional complexity that remain unmatched in synthetic systems. Despite substantial advances in the design of synthetic oligomers with well-defined conformations, encoding higher-order structural organization directly within their primary sequence remains a significant challenge.^{1,2}

As a first step toward this goal, the Cougnon group has previously demonstrated that the primary sequence of oligo(*m*-phenylene ethynylene) strands, composed of hydrophobic phenylene and charged pyridinium units, can direct the self-assembly of multistranded helices in water.³ This first level of sequence control allows access to a limited set of four states: right- and left-handed double and triple helices.

In this work, we introduce a second level of control through the incorporation of lateral side chains, which enables the selective amplification of a single structure within this set, the (*P*)-triple helix. We will show how the number of hydrogen bonding-units in the side chain and pH variation critically tune triple helix stability and diastereomeric excess highlighting a fine interplay between chiral transfer, geometric constraints and electrostatic interactions.

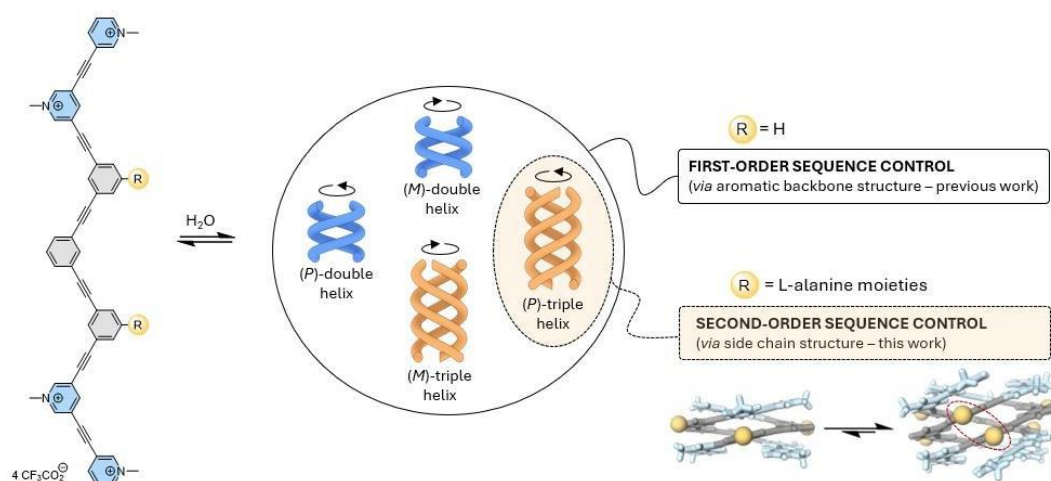


Figure 1: Hierarchical sequence design directs the self-assembly of a triple helix with preferred handedness.

¹ G. Ladevaia, J. A. Swain, D. Núñez-Villanueva, A. D. Bond, C. A. Hunter, *Chem. Sci.* **2021**, *12*, 10218-10226.

² Y. Liu, F. C. Parks, W. Zhao, A. H. Flood, *J. Am. Chem. Soc.* **2018**, *140*, 15477-15486.

³ D. Delcourt, R. Arumugaperumal, P. Verma, P. Perttu, R. M. Gomila, A. Frontera, F. B. L. Cougnon, *Nat. Commun.* **2025**, *16*, 10955.

Imidazole-Semicarbazones as Photo-Controllable Ion and Water Transporters

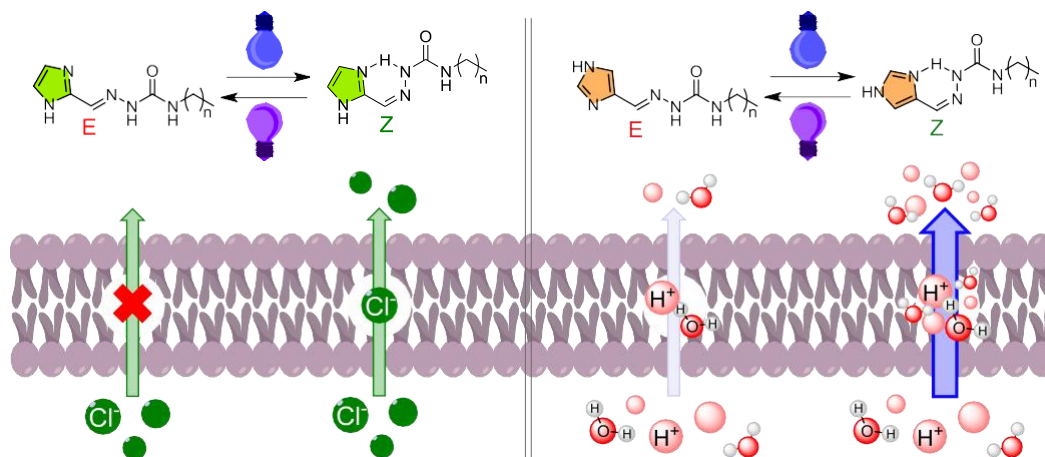
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Ion and water transport through the cell membrane is an essential process of cellular regulation, including pH control and osmotic pressure balance.^{1,2} While these transport phenomena open new perspectives to address diseases like cystic fibrosis,³ they can also lead to strong industrial applications in material science, for instance in the development of biomimetic desalinating membranes.⁴ In this context, a current objective lies in the design of controllable synthetic channels. Inspired by our previous works,^{5,6} we designed two new imidazole-based compounds now bearing photo-responsive semicarbazones, allowing for reversible E \leftrightarrow Z isomerization upon light irradiation (Figure 1). The two products were successfully synthesized and isolated as pure E and Z isomers. Their reversible photo-switching was studied in solution using ¹H NMR, HPLC and UV spectroscopy. Transport experiments in vesicles revealed different behaviors. In the first group where the imidazole is substituted at position 2 (Figure 1, left), the Z isomer showed a selective transport of chloride anion, while the E isomer had no transport activity. In the second group with the imidazole substituted at position 4 (Figure 1, right), the Z form displayed an increased water/proton transport, with salt exclusion, whereas the E form showed lower water/proton transport activity. In conclusion, this work has revealed fine relationships between the molecular design and transport phenomena, further documenting an example of photo-switchable ion and water transport using a new class of simple, versatile imidazole-semicarbazone transporters.



¹ Casey, J., Grinstein, S., Orlowski, J. *Nat. Rev. Mol. Cell. Biol.* **2010**, *11*, 50–61.

² Yan, T., Liu, J. *Angew. Chem. Int. Ed.* **2025**, *64*, e202416200.

³ Rathnaweera, U. M. C., Chowdhury, S. M., Salam, R., Busschaert, N. *Chem. Rev.* **2025**, *125*, 8370–8425.

⁴ Di Vincenzo, M., Tiraferri, A., Sougrat, R., Huang, L.-B., Nunes, S. P., Barboiu, M. *Nat. Nanotechnol.* **2021**, *16*, 190–196.

⁵ Wanjari, P., Stroia, I., van der Lee, A., Baaden, M., Barboiu, M. *J. Am. Chem. Soc.* **2025**, *147*, 39, 35264–35274.

⁶ Ulrich, S. *Acc. Chem. Res.* **2019**, *52*, 510–519.

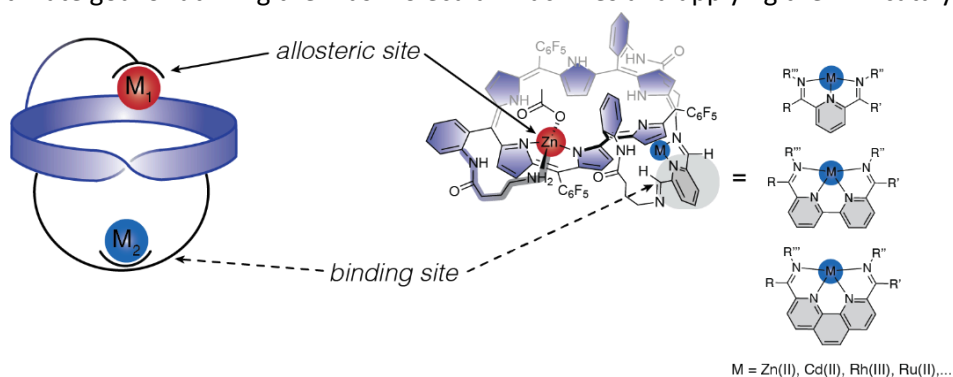
Möbius hexaphyrin with a metallo-allosteric site: interplaying a coordinating arm and coordinating strap

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All chiral molecules in nature, e.g., D-glucose, L-amino acids, and DNA play significant roles in chemical reactions involving chirality transfer, thereby controlling the outcome of substrates.¹⁻² These phenomena are usually observed in the roles of enzymes and receptors. Consequently, they have inspired the development of supramolecular systems for controlling the chemical reactions.³ The design of such molecules incorporates allosteric sites to receive the information and binding sites to perform the special tasks. Previously, our research team proposed the design of artificial supramolecular molecules based on hexaphyrin, which is composed of six pyrrole units. Hexaphyrin can adopt various conformations (Möbius, rectangular, triangular shapes), access different oxidation states, and exhibit both Hückel and Möbius aromaticity.⁴ The design based on Möbius aromatic hexaphyrin with covalent linkages of a TREN cap has been used for molecular recognition⁵, as well as hexaphyrin bearing chiral amino arms have been used for chirality induction.⁶ However, these Möbius hexaphyrins incorporated only a single coordination site.

Herein, we aim to synthesize Möbius hexaphyrins that combine both allosteric and binding sites within a single molecule. To achieve this, we proposed a design of Möbius hexaphyrins bearing an amino arm as the allosteric sites and pyridine derivative straps as the binding sites. As a result, we will form hexaphyrin complexes (mono- and bimetallic) through interactions with the pyridine derivative straps and study the chirality of these building block complexes, with ultimate goal of utilizing them as molecular machines and applying them in catalysis.



Acknowledgements Agence nationale de la recherche (ANR) - MOBAZYM

¹ M. Liu, L. Zhang, T. Wang, *Chem. Rev.* **2015**, *115*, 7304-7397.

² C. Liu, G. Fan, Z. Wang, H. Chen, C. Yin, *Sci Rep* **7**, **2017**, 1404 (1)-(9).

³ S. Cai, J. Chen, S. Wang, J. Zhang, X. Wan, *Angew. Chem. Int. Ed.* **2021**, *60*, 9686-9692.

⁴ T. Tanaka, A. Osuka, *Chem. Rev.* **2017**, *117*, 2584-2640

⁵ H. Ruffin, G. Nyame, M. Boussambe, T. Roisnel, V. Dorcet, B. Boitrel, S. Le Gac, *J. Am. Chem. Soc.* **2017**, *139*, 13847-13857.

⁶ T. Nédellec, B. Boitrel, S. Le Gac, *J. Am. Chem. Soc.* **2023**, *145*, 27067-27079.

Regioisomerism-Dependent Optoelectronic and Supramolecular Behaviour of BisAzaCoroneneDiimide *N*-oxides

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Polyaromatic structures are known to form stimuli-responsive supramolecular aggregates in solution and solid states. As such, derivatives of porphyrins, acenes or rylene diimides¹ are in the scope of supramolecular chemist due to their ability to engage in π -stacking leading to oligomers and polymers, which then affords new optical or electronic properties. In our group, we focus extensively on the π -extension of perylene diimide starting from amine-functionalized building-blocks.^{2,3} Recently, we have developed a strategy allowing the preparation of pristine bisazacoronene diimide (**1,6-** and **1,7-BACD**) through a simple procedure involving both oxygen and light as reagents and activation sources. The presence of molecular oxygen during the synthesis controls the cleavage or retention of the side-groups. The corresponding *N*-Oxide (**1,6-** and **1,7-BACDO₂**) present significant regioisomerism-dependent aggregation properties. While the **1,6-** isomer does not exhibit significant auto-association properties upon solvatochromic and thermal experiment, the **1,7-** one does, thus displaying bathochromic shifts in the presence of polar solvents. Moreover, the temperature dependence of the **1,7-BACDO₂** supramolecular assembly was investigated, highlighting a reversible thermal behaviour of the aggregation and revealing a supramolecular polymerization mechanism following a cooperative model.

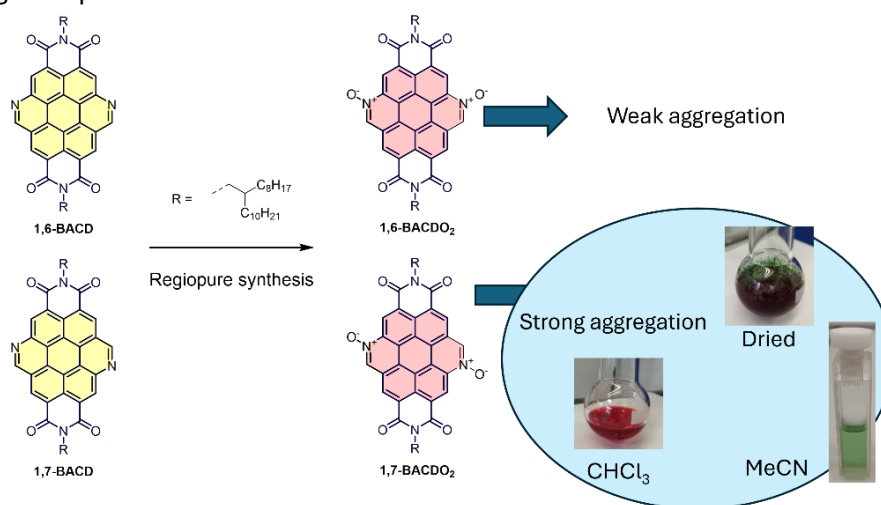


Figure 1. Isomers **1,6-** and **1,7-BACDO₂** and their aggregation properties in solution and solid state.

- (1) Wu, J.; Peng, M.; Mu, M.; Li, J.; Yin, M, *Supramolecular Materials* **2023**, *2*, 100031.
- (2) David, A. H. G.; Shymon, D.; Melville, H.; Accou, L.-A.; Gapin, A.; Allain, M.; Alévêque, O.; Force, M.; Grosjean, A.; Hudhomme, P.; Bras, L. L.; Goujon, A, *J. Mater. Chem. C* **2023**, *11* (42), 14631–14640.
- (3) David, A. H. G.; Roger, M.; Alévêque, O.; Melnychenko, H.; Le Bras, L.; Allain, M.; Gapin, A.; Canevet, D.; Ségut, O.; Levillain, E.; Goujon, A, *Angewandte Chemie International Edition* **2025**, *64* (1), e202413616.

Electron-Responsive Conductive Supramolecular Materials Based on Viologens Self-Assembly

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Thanks to their non-covalent nature, supramolecular gels obtained through the assembly of low molecular weight gelators (LMWGs) are highly stimuli-responsive materials (pH, T, P, light).¹ Redox-active supramolecular gels are highly promising soft materials for many applications ranging from catalysis to electronics.² Nonetheless, due to major scientific and technical challenges electrochemical stimulation of supramolecular gels still remains mostly unexplored.³⁻⁴ We recently described the synthesis and detailed characterizations of supramolecular gels obtained by self-assembly of a cholesteryl substituted viologen LMWG (Figure 1).⁵⁻⁶ Careful control over the formation of charge-transfer complexes between viologens and iodide ions have led to robust, translucent, conductive and chiral gels.⁵ This presentation will focus on the photo- and electrochemical stimulation of these viologen conductive gels and on the corresponding in operando characterizations (UV-vis, optical microscopy and coulometry). We will for instance show that the reduction of the viologen units triggers a gel→sol transition coming along with a collapse of the gel microstructure.⁷ Such phase transition could be obtained through both photochemical and electrochemical route. Electrochemical reoxidation of the viologen radicals allowed to reform gelator's dense supramolecular network, constituting one of the first examples of reversible supramolecular polymerization driven by an electrochemical output.⁷

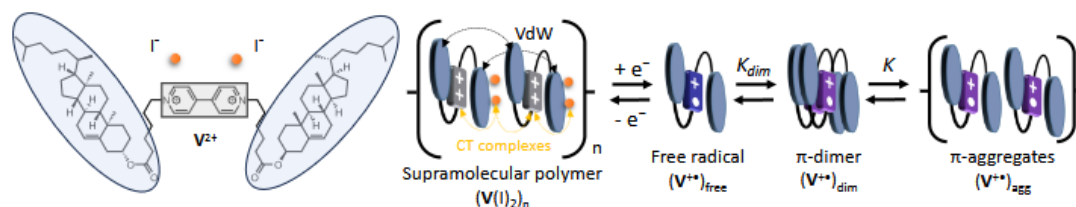


Figure 1 : Molecular structure of gelator V^{2+} (left) and scheme representing the different supramolecular reorganization steps triggered through electrochemical stimulation of the self-assembled system (right).⁷

Acknowledgements. CNRS and ENS de Lyon are acknowledged for continuous support. This work was supported by the ENS de Lyon with a CDSN PhD Grant, the LABEX iMUST (ANR-10-LABX-0064) of Université de Lyon within the program “Investissements d’Avenir” (ANR-11-IDEX-0007) (ANR), by the ANR ANGEL (ANR-21-CE06-0020), by the ANR ChiroSwitch (ANR-22-CE06-0012) and by the “Mission pour les initiatives transverses et interdisciplinaires” MITI CNRS (Auto-organisation AAP 2020).

¹ S. Panja and D. J. Adams, *Chem. Soc. Rev.*, **2021**, *50*, 5165; ² W. Guan, K. M. Adam, M. Qiu, Y. Zhang, H. Yao, T. Wei and Qi Lin, *Supramolecular Chemistry*, **2020**, *32:11*, 578-596A; ³ K. Hatakeyama-Sato and K. Oyaizu, *Chem. Rev.* **2023**, *123*, 19, 11336–11391; ⁴ R. I. Randle, A. M. Fuentes-Caparrós, L. P. Cavalcanti, R. Schweins, D. J. Adams, E. R. Draper, *J. Phys. Chem. C* **2022**, *126*, 31, 13427–13432; ⁵ V. Andrieux, T. Gibaud, J. Bauland, T. Divoux, S. Manneville, S. Guy, A. Bensalah-Ledoux, L. Guy, F. Chevallier, D. Frath and C. Bucher, *J. Mater. Chem. C*, **2023**, *11*, 12764-12775; ⁶ J. Bauland, V. Andrieux, F. Pignon, D. Frath, C. Bucher, and T. Gibaud, *Soft Matter*, **2024**, *20*, 8278-829; ⁷ V. Andrieux, R. Savin; T. Gibaud, J. Bauland, F. Chevallier, D. Frath and C. Bucher, *Chem. Eur. J.* **2025**, *31*, e02489.

Azacalixarene's Midlife Crisis: Cyanide Capture and Spontaneous Liberation

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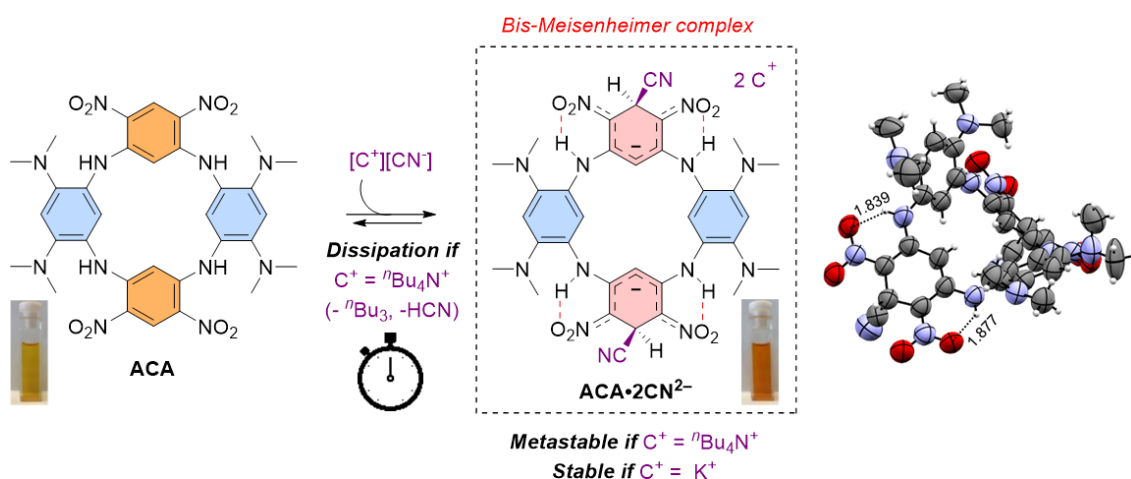
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Among heterocalixarenes, azacalixarenes (ACA) are of particular interest due to the presence of nitrogen bridges, which significantly impact their physicochemical properties. This makes them valuable scaffolds for applications ranging from ion sensing¹ to the development of porous covalent organic frameworks for dialysis and depollution.²

We recently designed an electron-deficient ACA that captures cyanide *via* a partial nucleophilic aromatic substitution process, forming a metastable dianionic macrocycle bearing two Meisenheimer units. Stabilized by intramolecular hydrogen bonding interactions, this bis-adduct can spontaneously dissociate under mild conditions to regenerate the parent macrocycle. The reversible, fuel-driven process establishes a rare example of a dissipative system, tunable by counterion, concentration, solvent, and temperature.³



¹ a) G. Canard, J. Andeme Edzang, Z. Chen, M. Chessé, M. Elhabiri, M. Giorgi, O. Siri, *Chem. Eur. J.* **2016**, *22* 5756; b) K. Salvadori, P. Matějka, P. Lhoták, O. Siri, *J. Org. Chem.* **2026**, *in press*.

² a) T. Skorjanc, D. Shetty, F. Gándara, S. Pascal, N. Naleem, S. Abubakar, L. Ali, A. K. Mohammed, J. Raya, S. Kirmizialtin, O. Siri, A. Trabolsi, *ACS Appl. Mater. Interfaces* **2022**, *14*, 39293; b) N. Elmerhi, K. Al-Maqdi, K. Athamneh, A. K. Mohammed, T. Skorjanc, F. Gándara, J. Raya, S. Pascal, O. Siri, A. Trabolsi, I. Shah, D. Shetty, S. S. Ashraf, *J. Hazard. Mater.* **2023**, *459*, 132261.

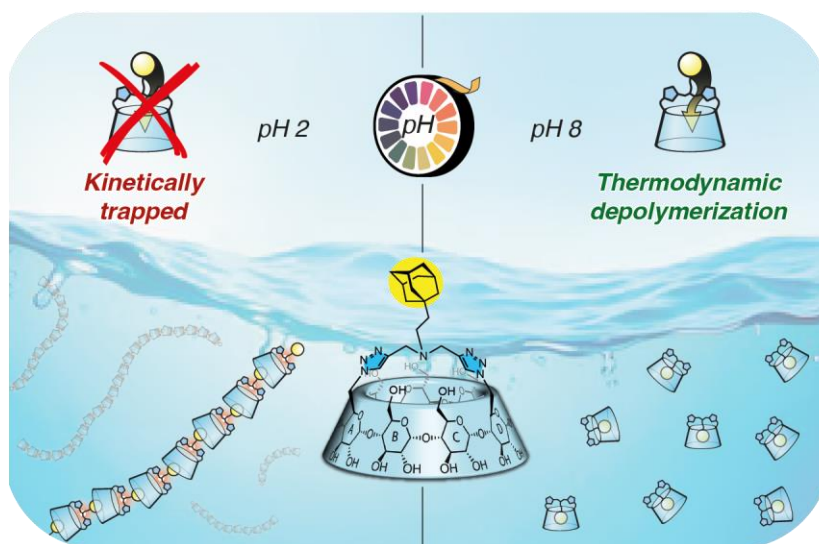
³ S. Pascal, A. Torres Ruiz, A. E. Baker, D. A. Vander Griend, M. Giorgi, A. Planchat, D. Jacquemin, O. Siri, *Angew. Chem. Int. Ed.* **2025**, *64*, e202511037.

pH-Gated Transient Supramolecular Polymerization of Cyclodextrins

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The binding of a cyclodextrin (CD) host to a hydrophobic guest results in either an introverted (in) form, where the guest self-includes in the CD cavity, or an extraverted (out) form, allowing supramolecular polymerization. When self-inclusion occurs, it usually leads to a dead end, as self-inclusion is generally the most thermodynamically stable conformation. We therefore developed a bridged cyclodextrin that prevent the hydrophobic side-group from self-inclusion and then demonstrated that this design generates isodesmic supramolecular polymers. In this contribution,¹ we have developed another bridging motif in which the hydrophobic group occupies a central position. This subtle modification of the bridging provides sufficient flexibility to lead, in water, to self-inclusion of the hydrophobic group despite the bridging. However, unlike conventional self-included cyclodextrin systems, the extraverted conformer can be restored and kinetically trapped, thus allowing supramolecular polymerization. In this presentation, we will reveal how the nature of the solvent and the pH can be adjusted to control the interconversion of both conformational states and, consequently, the transient nature of the polymerization process.



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¹ W. Hu, V. Libérioux, J. Rossignol, G. Pembouong, E. Derat, M. Ménand, L. Bouteiller, M. Sollogoub, *Angew. Chem. Int. Ed.* **2025**, e202507069.

Supramolecular Confinement Enables Selective CO₂-to-CO Conversion in Water

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Electrocatalytic CO₂ reduction (CO₂RR) has emerged as a promising, sustainable strategy for converting CO₂ into fuels and value-added chemicals, while harnessing intermittent renewable energy sources.¹ However, CO₂RR is a complex process involving multiple proton- and electron-transfer steps, which can yield a variety of products (e.g., CO, HCOO⁻, CH₄, CH₃OH) and undesired side reactions, such as the hydrogen evolution reaction (HER).²

Inspired by natural enzymes, where catalytic sites are spatially confined and surrounded by a tailored environment to achieve optimized activity, we developed a confined system in which the well-known manganese bipyridine electrocatalyst, [Mn(bpy)(CO)₃(CH₃CN)]⁺,³ is encapsulated within a silicon-based metal-organic cage, via a host-guest strategy involving electrostatic interactions.

When immobilized on multi-walled carbon nanotubes (MWCNTs), this confined system exhibits outstanding electrocatalytic performance for CO₂RR in aqueous 0.5 M KHCO₃ solution, achieving a faradic efficiency for CO production exceeding 90%, in contrast to ~30% observed for the free catalyst. Moreover, the assembly shows enhanced durability, maintaining catalytic activity and CO selectivity for at least 6 hours at -1.29V vs Ag/AgCl. The exact CO₂RR mechanism for this confined system is currently under investigation in our laboratory. ATR-IR spectroelectrochemical experiments in aqueous media suggest the formation of a Mn⁰ intermediate species and the prevention of dimerization. DFT calculations allow us to rationalize the reaction selectivity on the basis of the stabilization of the Mn-carboxylate intermediate by the organosilicate functional groups of the cage.

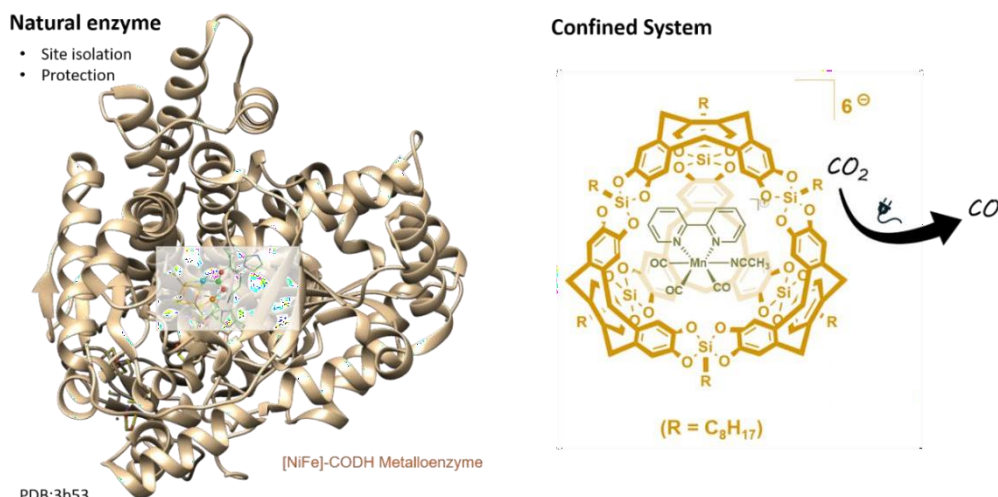


Figure 1: [NiFe]-CODH metalloenzyme (left). Confined system studied in this work (right)

¹ S. Van Renssen, Nature Climate Change 2020, 10, 799-801

² N. W. Kinzel, C. Werlé, W. Leitner, Angew. Chem. Int. Ed. 2021, 60, 11628-11686.

³ M. Bourrez, F. Molton, S. Chardon-Noblat, A. Deronzier, Angew. Chem. Int. Ed. 2011, 50, 9903-9906.

Self-Assembled Organometallic Cages from poly-NHC Perylenebisimide Based Ligands

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Organometallic assemblies based on N-Heterocyclic carbene ligands (NHC) possess strong metal-carbon bonds enabling chemical and thermal stability.¹ However, the confined nanospaces offered by the existing NHC-based assemblies neither allow relevant molecular recognition nor catalytic activity.² To tackle this bottleneck, our group aims at the synthesis of a unique family of NHC-self-assembled assemblies featuring electrodefficient perylenebisimide (PBI) allowing for tunable confined nanospaces that may find applications in mixed-valence species, energy transfer or catalysis.

Several analytical techniques allowed us to confirm the molecular structure of the assemblies, as well as their stability. We will thus present the multi-step synthesis of two perylenebisimide ligands, and their narcissistic self-assembly to form four metallacages either assembled with Ag^I or Au^I metal ions.

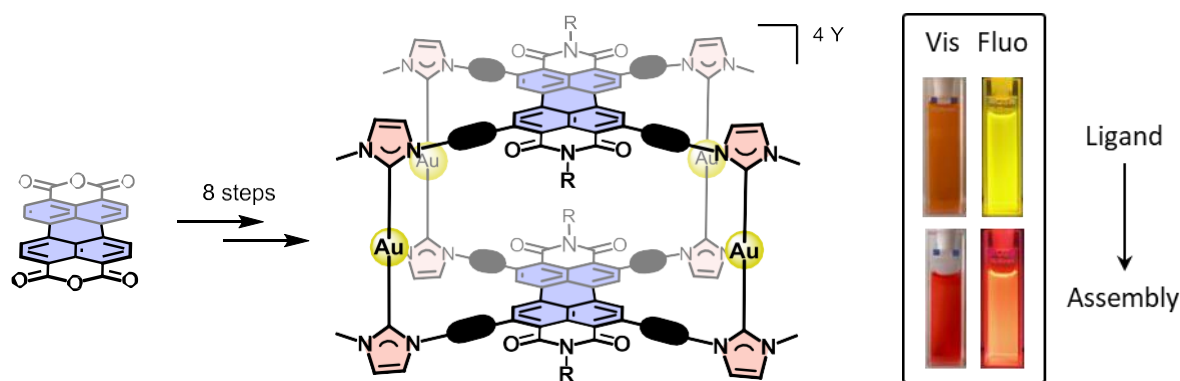


Figure 1. Representation of the organometallic cages obtained from poly-NHC perylenebisimide based ligand

Acknowledgements. Laboratory iSm2-Marseille and Ecole Centrale Méditerranée for installation grants & Lorraine University for young researchers fellowship (call 2025).

¹ M. M Gan, J. Q. Liu, L. Zhang, Y. Y. Wang, F. Ekkehardt Hahn, and Y. F. Han; *Chem. Rev.* **2018**, *118*, 9587

² S. R. Thomas, N. Willnhammer, A. Casini, and G. Moreno-Alcantar; *Chem.* **2025**, *11*, 102502

Flash communications



Caged Macrocycles: Towards non-heme bioinspired catalysts

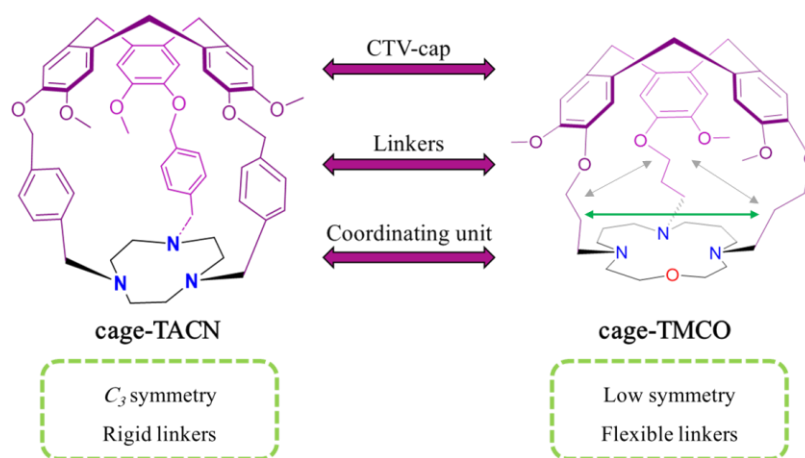
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Metalloenzymes are biocatalysts that catalyse difficult reactions with remarkable selectivity and efficiency. Cyclic polyamine ligands such as 1,4,7-triazacyclononane (**TACN**) and 1-oxa-4,8,12-triazacyclotetradecane (**TMCO**) are known for their ability to bind metal cations to form bioinspired catalysts.^[1,2] For instance, open Cu(I) **TACN**-based complexes can activate O₂ to produce powerful oxidizing species.^[3] Furthermore, Fe(II) **TMCO**-based complexes were used as model compounds for the study of oxygenases' mechanism.^[2]

However, in order to mimic metalloenzyme's activity, and improve the selectivity and efficiency of artificial catalysts, it is crucial to not only replicate the first coordination sphere, but also mimic the hydrophobic cavity surrounding the active site. To do so, it is possible to build supramolecular cages around artificial bioinspired complexes.

In particular, the cyclotrimeratrylene (**CTV**)-based hemicryptophane cage-ligands, have been used in our group enabling advanced catalysts and receptors (e.g., CH₄ oxidation).^[4] The goal of this work therefore is to reach unprecedented **TMCO** ligand and Cu(I)**TACN** complex equipped with hydrophobic cavities (Scheme 1). In particular, **cage-TMCO** displays a low symmetrical cavity offering 3 differently sized windows, getting closure to the low-symmetrical enzymatic cavities. Herein, the synthesis of two **TACN**- and one **TMCO**-based cages, displaying well-defined cavities of varying volumes and flexibility, is presented along with the study of their corresponding Cu(I) complexes as potential O₂ activating confined catalysts.



Scheme 1 Structure of the **TACN**-based caged (left) and structure of the **TMCO**-based caged ligand (right)

[1] R. Tripier, *et al. Inorg. Chem.* **2019**, 2669.

[2] K. Ray, *et al. Nat. Chem.* **2024**, 16 (4), 658–665.

[3] W. B. Tolman, *et al. Science* **1996**, 1397.

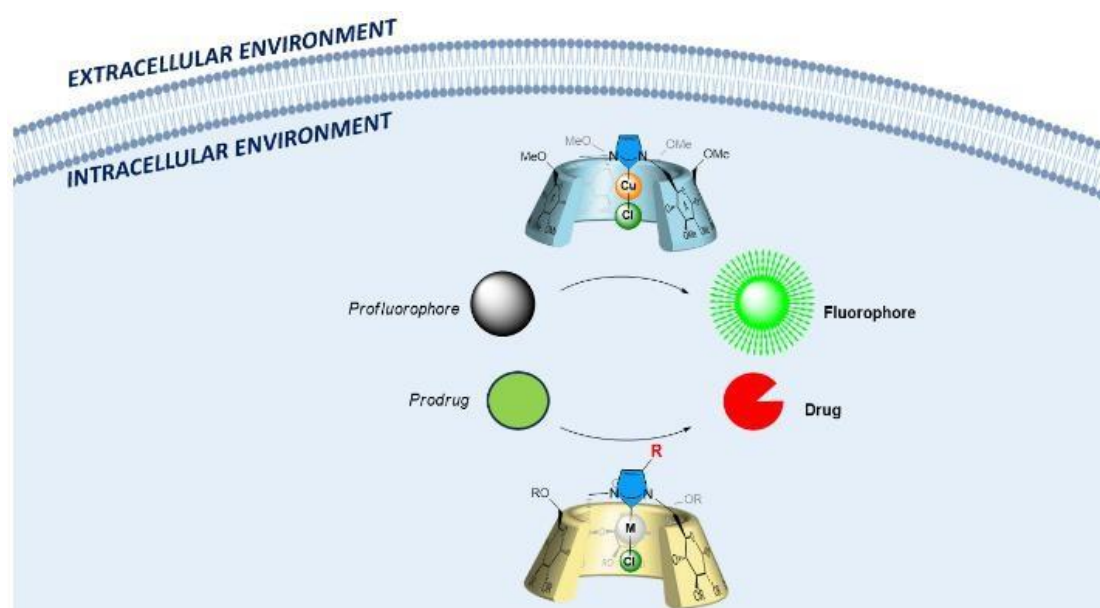
[4] (a) C. Colombar, *et al. Chem. Commun.* **2023**, 4288. (b) C. Colombar, *et al. JACS Au* **2024**, 1966

Metal complexes based on modified cyclodextrins for the development of catalytic reactions in cells

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The use of organometallic catalysis in living cells offers promising avenues for imaging (via profluorophores) and therapeutic applications (via prodrugs). While most systems rely on rare and precious metals, copper(I) complexes represent an appealing alternative due to copper abundance and versatile reactivity.¹ However, intracellular copper catalysis face key challenges: metal toxicity, cellular uptake, competition with endogenous copper pools, stability, compatibility with complex cell media, and the need for biocompatible activation wavelengths in the case of photoactivation. Our group previously developed NHC-based metal complexes (Ag, Cu, Au, etc.),^{2,3,4} encapsulated in cyclodextrins (CDs), which protect the catalyst and preserve its catalytic activity while suppressing cytotoxicity. Building on this, we were able to carry out *ipso*-hydroxylation reactions of boronic esters in DMEM cell culture medium and in cancer cells, by using water-soluble NHC–copper complexes encapsulated in CDs, demonstrating their compatibility with complex biological environments. We now aim to adapt this system for cellular applications by improving cell permeability, enhancing intracellular copper competition, and by testing more stable NHC-based metal complexes—especially gold-based ones—to explore new orthogonal reactivities in cells.



- (1) Madec, H.; Figueiredo, F.; Cariou, K.; Roland, S.; Sollogoub, M.; Gasser, G. *Chem. Sci.* **2023**, *14*, 409–442.
- (2) Guitet, M.; Zhang, P.; Marcelo, F.; Tugny, C.; Jiménez-Barbero, J.; Buriez, O.; Amatore, C.; Mouriès-Mansuy, V.; Goddard, J.; Fensterbank, L.; Zhang, Y.; Roland, S.; Ménand, M.; Sollogoub, M. *Angew Chem Int Ed* **2013**, *52*, 7213–7218.
- (3) Zhang, P.; Mejjide Suárez, J.; Driant, T.; Derat, E.; Zhang, Y.; Ménand, M.; Roland, S.; Sollogoub, M.. *Angew. Chem Int Ed* **2017**, *129*, 10961–10965.
- (4) Zhu, X.; Xu, G.; Chamoreau, L.; Zhang, Y.; Mouriès-Mansuy, V.; Fensterbank, L.; Bistri-Aslanoff, O.; Roland, S.; Sollogoub, M. *Chem. Eur J* **2020**, *26* (68), 15901–15909.

Elaboration of non fullerene acceptors for Indoor Photovoltaics

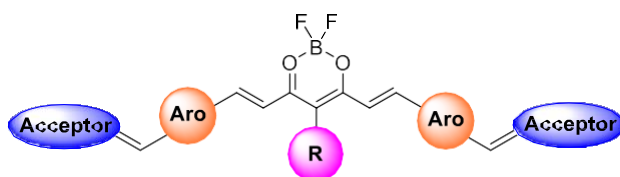
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Organic solar cells (OSCs) are light, flexible and easy to produce, with energy conversion efficiencies up to 19 %¹. However, they are not widely used for applications with artificial lighting, and their performance is limited, partly due to the use of fullerenes and their derivatives as electron acceptors in the active layer². To overcome these limitations, in this project, we are looking at curcuminoid derivatives to use them as non fullerene acceptors (NFAs). Curcumin is the main molecule of *Curcuma longa* L., also known as turmeric and has been used for centuries as a natural dye³ and for its medicinal properties⁴. These last decades, curcumin is also studied for its photophysical properties⁵ due to its 1,3-diketone core and its π -conjugated skeleton. Curcuminoid derivatives with a boron difluoride complex were synthesized to improve the curcumin photophysical properties⁶, and are mainly used as fluorescent tags, in optoelectronics⁷ like in OLEDs⁸, but also in OSCs. Archet *et al.*⁹ synthesized a curcuminoid derivative used as an electron donor in the active layer of OSCs, with power conversion energy up to 4.14 % and a high open-circuit voltage over 1.0 V, when associated with PC61BM.

This project focuses on the development of a new family of NFAs: curcuminoid derivatives with a boron difluoride complex, whose structures are inspired by known NFAs. These compounds are synthesized and then characterized (UV-Vis absorbance, cyclic voltammetry, applications in OSCs).



General structure of curcuminoid derivatives as NFAs

¹ National Laboratory of the Rockies. *Best Research-Cell Efficiency Chart | Photovoltaic Research | NLR*.

² Xu, X.; Liu, W.; Luo, X.; Chen, H.; Wei, Q.; Yuan, J.; Zou, Y. *ChemSusChem* **2021**, *14* (17), 3428–3448.

³ Ravindran, P. N.; Babu, K. N.; Sivaraman, K. **2007**.

⁴ Lee, W.-H.; Loo, C.-Y.; Bebawy, M.; Luk, F.; Mason, R.; Rohanizadeh, R. *Curr. Neuropharmacol.* **2013**.

⁵ Benassi, R.; Ferrari, E.; Lazzari, S.; Spagnolo, F.; Saladini, M. *J. Mol. Struct.* **2008**, *892* (1–3), 168–176.

⁶ Ran, C.; Xu, X.; Raymond, S. B.; Ferrara, B. J.; Neal, K.; Bacskai, B. J.; Medarova, Z.; Moore, A. *J. Am. Chem. Soc.* **2009**, *131* (42), 15257–15261.

⁷ D'Aléo, A.; Zaborova, E.; Fagès, F. *Tech. Ing.* **2018**.

⁸ Gál, E.; Nagy, L. C.; Gál, E.; Nagy, L. C. *Symmetry* **2021**, *13* (12).

⁹ Archet, F.; Yao, D.; Chambon, S.; Abbas, M.; D'Aléo, A.; Canard, G.; Ponce-Vargas, M.; Zaborova, E.; Le Guennic, B.; Wantz, G.; Fages, F. *ACS Energy Lett.* **2017**, *2* (6), 1303–1307.

Porphyrin cages for photoredox catalysis of heterobiaryls

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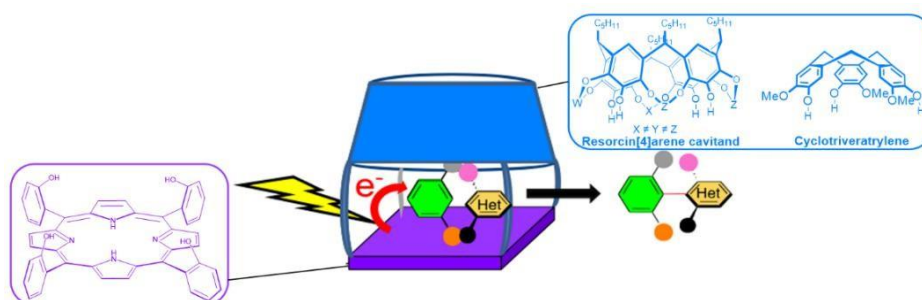
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Molecular cages are discrete compounds with cavities that can encapsulate smaller molecules through non-covalent interactions. They are designed for applications in molecular recognition, transport or catalysis. In supramolecular catalysis, they have demonstrated abilities to accelerate reactions, like Diels-Alder¹, and induce regio- and stereo-selectivity,² for example in the photodimerization of olefins.³ Recently, molecular cages with light-absorbing properties have emerged as promising systems for photocatalysis.^{4,5} However, metal-free covalent organic cages remain less explored than coordination cages, due to the need to integrate a photoactive unit.

In this project, new metal-free cages of different shapes and sizes are designed for supramolecular photoredox catalysis of enantioselective formation of heterobiaryls. These cages integrate a free-base porphyrin linked to a chiral concave capping unit: a cyclotrimeratrylene (CTV) or a resorcin[4]arene-based phosphonate cavitands (P-CAV). This design combines the photoredox activity of a porphyrin⁶ with the ability of the bowl-shaped component to stabilize encapsulated cations and neutral guests.⁷ Herein, we describe the synthesis of a CTV-porphyrin cage with triazole linkers by a templated approach and the preliminary results of the photoredox catalysis.



Porphyrin cages for the photoredox coupling of aryls diazonium salts and heteroarenes.

Acknowledgements. The ANR (ANR-23-CE07-0035 AtropoPhotoCat) and the GDR MAPYRO are gratefully acknowledged.

¹ M. Yoshizawa, M. Tamura, M. Fujita, *Science* **2006**, *312*, 251–254.

² M. Morimoto, S. M. Bierschenk, K. T. Xia, R. G. Bergman, K. N. Raymond, F. D. Toste, *Nat. Catal.* **2020**, *3*, 969–984.

³ M. Yoshizawa, Y. Takeyama, T. Kusakawa, M. Fujita, *Angew. Chem. Int. Ed.* **2002**, *41*, 1347–1349

⁴ R. Ham, C. J. Nielsen, S. Pullen, J. N. H. Reek, *Chem. Rev.* **2023**, *123*, 5225–5261.

⁵ S. Tanaka, T. Nakazono, K. Yamauchi, K. Sakai, *Chem. Lett.* **2017**, *46*, 1573–1575.

⁶ D. Gryko, K. Rybicka-Jasińska, B. König, *Eur. J. Org. Chem.* **2017**, *2017*, 2104–2107.

⁷ D. Zhang, A. Martinez, J.-P. Dutasta, *Chem. Rev.* **2017**, *117*, 4900–4942

Not going back: Unidirectional movement by intramolecular one-way ratcheting of functionalized cyclodextrin

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Molecular motion is vital for life, driving essential processes at the nanoscale within living cells. This is made possible by biomolecular motors, which can perform unidirectional motion. For example, kinesin motor proteins transport cargos along microtubules.¹ Such directional movement arises from biasing Brownian motion through chemically fueled Brownian ratcheting mechanisms.² Natural systems have inspired scientists to design artificial molecular motors.³ While unidirectional motion has been achieved using information ratchet mechanisms in rotaxanes and catenanes,^{4,5} exploiting the intrinsic asymmetry of a three-dimensional macrocycle to drive motion via ratcheting remains unexplored.

In this work, we present an information ratchet that exploits the inherent asymmetry of cyclodextrin's cone-shaped macrocycle to achieve directional motion in a rotaxane. By selectively functionalizing the cyclodextrin small rim, we enable a mechanospecific deprotection of temporary stoppers positioned on the rotaxane axle in front of the CD. As a result, under chemical fueling, the CD moves autonomously in a single direction by opening the stoppering gates exclusively one way, and subsequently favoring their closure⁶ once it has passed through. This system demonstrates a synergistic, double-gated, one-way ratchet mechanism driven by the unique asymmetrical structure of the cyclodextrin paving the way toward long-range linear molecular motors (Figure 1).⁷

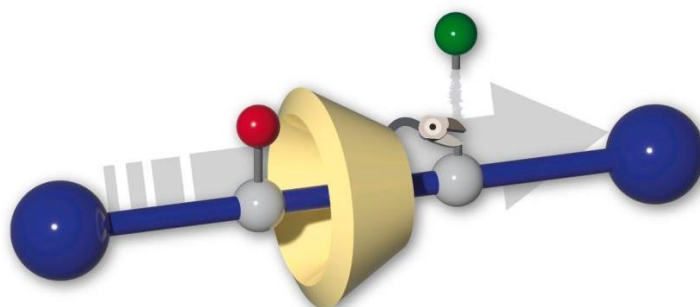


Figure 1. Schematic representation of the double-gated one-way ratcheted system.⁷

¹N. Hirokawa, Y. Noda, Y. Tanaka, S. Niwa, *Nat. Rev. Mol. Cell Biol.* **2009**, *10*, 682–696.

²M. Schliwa, G. Woehlke, *Nature* **2003**, *422*, 759–765.

³S. Erbas-Cakmak, D. A. Leigh, C. T. McTernan, A. L. Nussbaumer, *Chem. Rev.* **2015**, *115*, 10081–10206.

⁴Y. Ren, R. Jamagne, D. J. Tetlow, D. A. Leigh, *Nature* **2022**, *612*, 78–82.

⁵M. R. Wilson, J. Solà, A. Carlone, S. M. Goldup, N. Lebrasseur, D. A. Leigh, *Nature* **2016**, *534*, 235–240.

⁶E. Liu, S. Cherraben, L. Boulo, C. Troufflard, B. Hasenknopf, G. Vives, M. Sollogoub, *Chem* **2023**, *9*, 1147–1163.

⁷E. Liu, D. Daou, B. Hasenknopf, G. Vives, M. Sollogoub, *Chem* **2025**, 102623.

Low-Symmetry Hemicryptophanes functionalized with Azaphosphatrane derivatives

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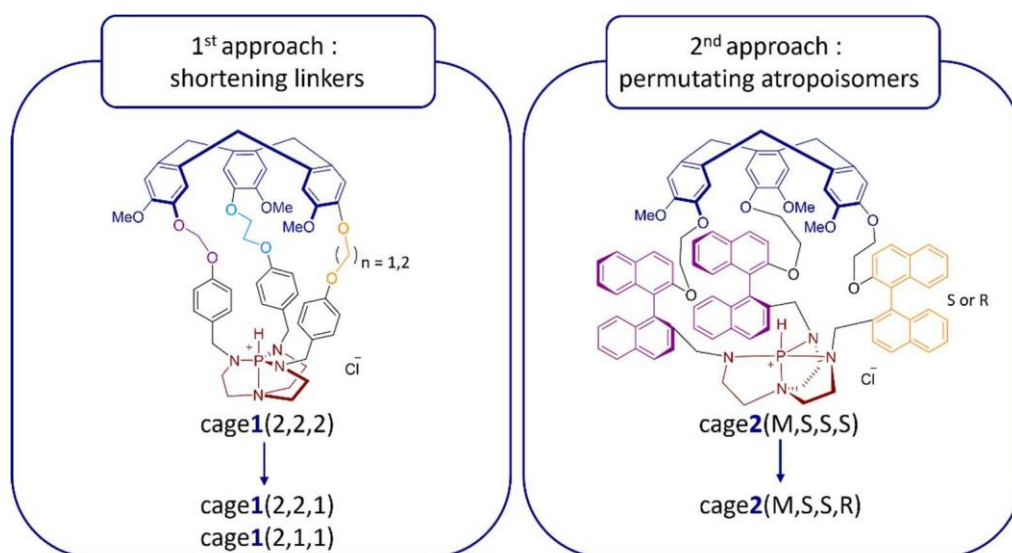
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Azaphosphatranes (in red in Scheme below) are pro-azaphosphatrane's acidic counterparts, stable species that could be used to generate reactive **pro-azaphosphatranes** in a single step.¹ The latter, also known as Verkade's superbases, were discovered in 1989 by Verkade. These species are highly basic with a pKa around 32 in CH₃CN. Pro-azaphosphatranes have been used as basic and nucleophilic catalysts in various transformations, such as isocyanurate formation or Strecker reaction.²

Previously in the team³, we reported an endohedral functionalized cage displaying catalytic activity in **base-catalysed Diels-Alder reaction** between prochiral 3-hydroxy-2-pyrone and various dienophiles through activation with encaged pro-azaphosphatrane as base. The crucial role of the molecular cavity on catalytic performance was highlighted.

On this basis, the objective is to access **low-symmetry endohedral cages** (Scheme below) using two innovative methods, thus enabling better substrate selectivity and diastereoselectivity. One aspect of this work deals with the tuning of linkers' length to functionalize the azaphosphatrane moiety with the enantiopure **CTV cap** (Scheme, left). Another approach uses three enantiopure 1,1'-binaphthyl linkers, creating a highly chiral hemicryptophane cage 2 (Scheme, right) for enantioselective catalysis. Cage syntheses will be presented with the study of corresponding pro-azaphosphatrane bases as catalysts.



Acknowledgements. This project has been carried out with the financial support of the A*MIDEX (no. AMX-22-RE-AB-141), funded by the Investissements d'Avenir project of the French Government (ANR).

¹ B. A. D'S, J. G. Verkade, *J. Org. Chem.* **1996**, *61* (9), 2963–2966

² J. G. Verkade, P. B. Kisanga, *Tetrahedron* **2003**, *59* (40), 7819–7858

³ Chatelet, B., Dufaud, V., Dutasta, J.-P. & Martinez, A. *J. Org. Chem.* **2014**, *79* (18), 8684–8688

Ordered Honeycomb Host–Guest Networks on HOPG for Supported Asymmetric Catalysis

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^[b] Institut de Chimie Moléculaire et des Matériaux d'Orsay, 91400, Orsay, France

Although heterogeneous catalysis offers clear advantages in terms of catalyst recovery and reuse, achieving high efficiency and cooperative effects between catalytic units remains difficult, especially for asymmetric transformations. Here, we aim to develop an ordered catalytic platform for the asymmetric hydrolysis of small meso-epoxides using salen complexes.

Our approach relies on the self-assembly of 3,5-Tri-(*E*)-styrylbenzene (TSB) on graphene to form a two-dimensional honeycomb-like molecular sieve¹. This supramolecular monolayer generates regular pores capable of accommodating polyaromatic species through non-covalent interactions². We propose to exploit this host–guest architecture to position pyrene-functionalized salen catalysts³ within the pores, thereby controlling their spatial arrangement at the surface. By tuning the inter-catalyst distance, we seek to reproduce the cooperative behavior previously observed between paired salen units⁴, with the goal of enhancing both enantioselectivity and reaction kinetics.

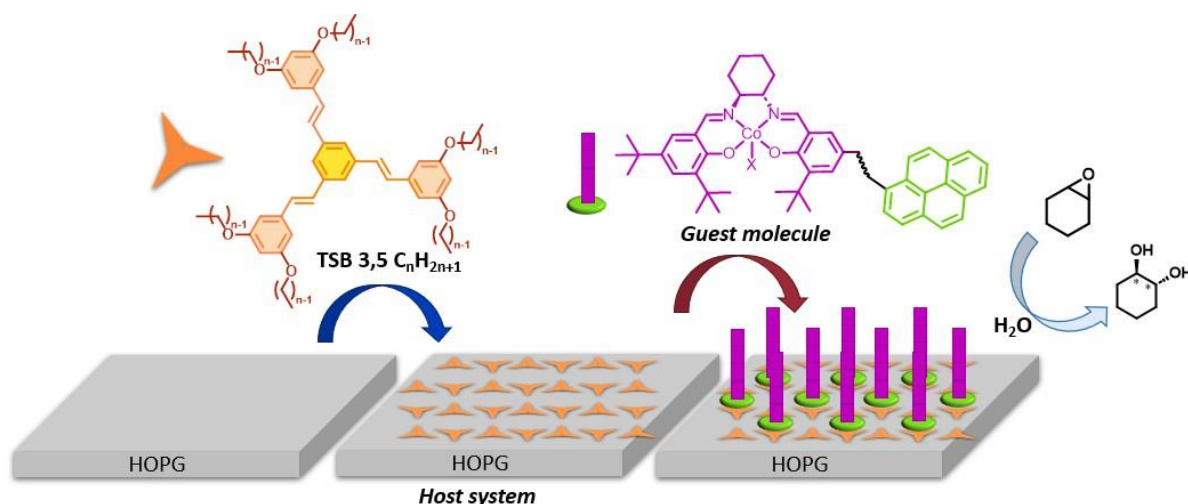


Figure 1. Hosting of pyrene-tagged Co-salen catalyst into the pores of the honeycomb system formed by the self assembly of TSB on graphene

¹ Bléger, D.; Kreher, D.; Mathevet, F.; Attias, A.-J.; Schull, G.; Huard, A.; Douillard, L.; Fiorini-Debuischert, C.; Charra, F. *Surface, Angew. Chem. Int. Ed.* **2007**, *46* (39), 7404–7407

² Schull, G.; Douillard, L.; Fiorini-Debuischert, C.; Charra, F.; Mathevet, F.; Kreher, D.; Attias, A.-J., *Adv. Mater.* **2006**, *18* (22), 2954–2957

³ Abd El Sater, M.; Mellah, M.; Dragoie, D.; Kolodziej, E.; Jaber, N.; Schulz, E., *Chem. – Eur. J.* **2021**, *27* (36), 9454–9460

⁴ Ready, J. M.; Jacobsen, E. N., *J. Am. Chem. Soc.* **2001**, *123* (11), 2687–2688

Chiroptical bis-(acridinium-Zn(II)porphyrin) Tweezers

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Porphyrins are known as excellent chromophores and fluorophores whose optical properties can be tuned by metal coordination.¹ These features make metalloporphyrins highly attractive for the chiroptical detection of non-absorbing chiral coordinating substrates. In particular, the close spatial arrangement of two porphyrin units can lead to a pronounced exciton coupling in the visible range.² Our group has explored the pH switching of acridinium units coupled to porphyrins in a tweezer architecture, and has recently demonstrated the possibility of switching the porphyrin luminescence in an on/off manner.³ We are now focusing on developing novel switchable acridinium-metalloporphyrin systems to investigate the chiroptical detection of substrates upon commutation, using both exciton-coupled circular dichroism (ECCD) and circularly polarized luminescence (CPL).⁴ In this context, we have synthesized two different bis-(acridinium-Zn(II)porphyrin) tweezers, which enable sensitive and intense chiroptical detection in the visible range (Figure 1).

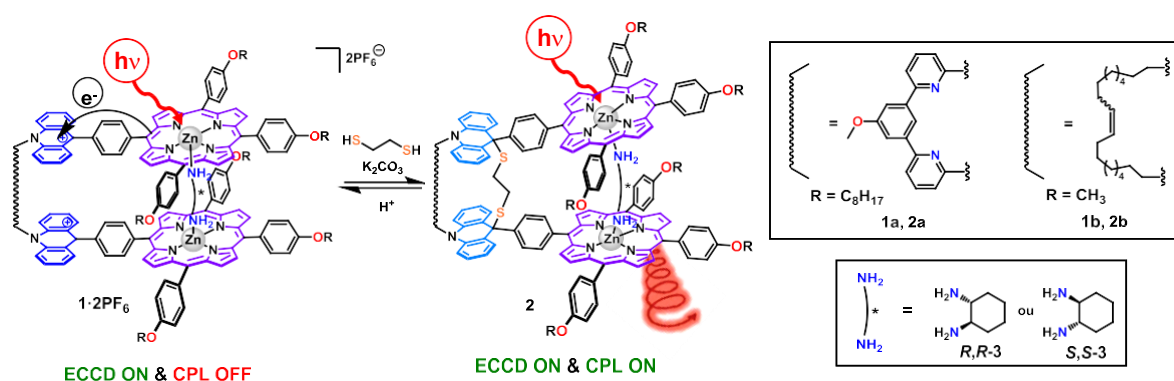


Figure 1. Chiral diamine recognition by a bis-(acridinium-Zn(II)porphyrin) tweezer and his luminescence switching properties

Acknowledgements. We would like to thank the University of Strasbourg, the CNRS, and the ENS Paris-Saclay for their financial support. This work was supported by the Interdisciplinary Thematic Institute SysChem via the IdEx Unistra (ANR-10-IDEX-0002) within the program Investissement d'Avenir ».

¹ A. R. Sekhar, Y. Chitose, J. Janoš, S. I. Dangoor, A. Ramundo, R. Satchi-Fainaro, P. Slaviček, P. Klán, R. Weinstain, *Nat. Commun.* **2022**, *13* (1), 3614.

² X. Huang, B. H. Rickman, B. Borhan, N. Berova, K. Nakanishi, *J. Am. Chem. Soc.* **1998**, *120* (24), 6185–6186.

³ 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* (19), 10691–10699.

⁴ K. Dhbaibi, P. Matozzo, L. Abella, M. Jean, N. Vanthuyne, J. Autschbach, L. Favereau, J. Crassous, *Chem. Commun.* **2021**, *57* (82), 10743–10746.

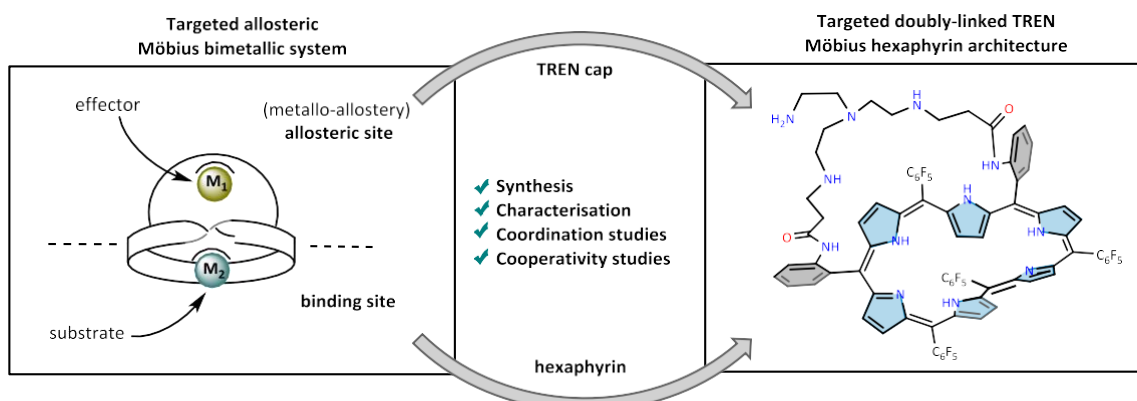
Möbius hexaphyrins with an overhanging metal binding site as unprecedented allosteric receptors

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Biomimicking has always been of great interest for decades. Nature shows remarkable specificity in metal involved biochemical processes through properties like allostery. Allostery involves the conformational change caused due to the effect on the allosteric site which in turn affects the affinity of the binding site. This specific property has been ubiquitous in enzymes and receptors.¹ To attain this kind of specificity, expanded porphyrins would be suitable platforms due to their fascinating properties such as topology, π -conjugation, coordination behaviour, aromaticity and reactivity.² The engineering of molecular receptors based on expanded porphyrins is quite under explored and challenging. From the previous work in our group, an hexaphyrin with a triply-linked TREN [tris(2-aminoethyl) amine] cap was proved to be a molecular host with a confined space accommodating a metal at the level of the Möbius hexaphyrin N-core, thereby enabling the binding of two guest molecules.³ In this work, we have improved our design and synthesized a Möbius hexaphyrin which is doubly-linked to the TREN cap. A free amino arm enables the metal coordination both at the level of the hexaphyrin as well as in the TREN, giving a bimetallic Zn (II) complex. The coordination of the metal at the level of TREN modifies the binding environment at the hexaphyrin N-core for the guest molecules (Hückel antiaromatic to Möbius aromatic conversion). This unique behaviour exhibited by the complex makes it an appropriate candidate for the further studies of allostery in Möbius type-receptors. To our knowledge, this is the very first example of a Möbius ring with an overhanging metal binding site.



Acknowledgements. The University of Rennes is acknowledged for the financial support.

¹ Kovbasyuk, L. & Krämer, R. Allosteric Supramolecular Receptors and Catalysts. *Chem. Rev.* **104**, 3161–3188 (2004).

² Tanaka, T. & Osuka, A. Chemistry of meso -Aryl-Substituted Expanded Porphyrins: Aromaticity and Molecular Twist. *Chem. Rev.* **117**, 2584–2640 (2017).

³ Ruffin, H. *et al.* Tren-Capped Hexaphyrin Zinc Complexes: Interplaying Molecular Recognition, Möbius Aromaticity, and Chirality. *J. Am. Chem. Soc.* **139**, 13847–13857 (2017).

Insights into self-assembly mechanisms and electrical properties of tetrazine-based supramolecular polymers

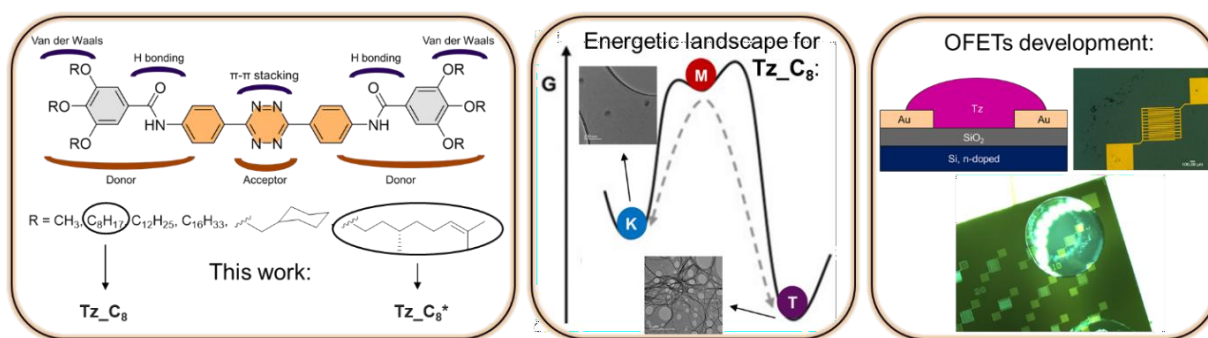
Lucrezia Trevisan,^[a,b] William T. Gallonde,^[a] Zuchong Yang,^[b] Vincent Dorcet,^[a] Arnaud Saint-Jalmes,^[c] Emanuele Orgiu,^[b] Stéphane Rigaut,^[a] Olivier Galangau*^[a]

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Supramolecular polymers are composed of monomeric units held together by highly directional and reversible secondary non-covalent interactions, resulting in dynamic species that can exhibit properties such as self-healing functions and responsiveness towards external stimuli.¹ Originally, supramolecular polymerization was regarded as a process entirely driven by thermodynamics. However, as the understanding of this process broadened, kinetic contributions started to emerge as impactful factors towards the outcome of the self-assembly, and multiple pathways in competition for the same monomer can occur. In particular, experimental conditions (*e.g.*, temperature or solvent modulation) and specific interactions (*e.g.*, donor-acceptor interactions) can have significant impact on the polymerization.^{2,3} We recently developed a new family of supramolecular polymers, featuring a central tetrazine core and different aliphatic side chains, resulting in donor-acceptor-donor structures with interesting self-assembly mechanisms. In determined conditions, supramolecular gels can be obtained, and given the electron properties (*e.g.*, available reduction potentials, electron deficiency) exhibited by tetrazine, these materials can be studied towards the development of novel n-type organic semiconductors.⁴ In this work, the self-assembly of two of these platforms (**Tz_C₈** and **Tz_C₈***) is explored, describing how subtle structural differences can not only impact the morphologies of these systems, but also their evolution towards thermodynamic equilibrium. Additionally, preliminary studies on their conductive capabilities are reported, with the development of organic field effect transistors (OFETs) featuring the tetrazine-based supramolecular gels.



¹ T. F. A. De Greef et al., *Chem. Rev.* **2009**, *109*, 5687–5754.

² J. Matern et al., *Angew. Chem. Int. Ed.* **2019**, *58*, 16730 – 16740.

³ F. Wang et al., *Angew. Chem. Int. Ed.* **2023**, *62*, e202305827.

⁴ G. Clavier, P. Audebert, *Chem. Rev.* **2010**, *110*, 3299–3314.

Mechanical disruption of β -Amyloid fiber analogs by out-of-equilibrium operation of light-driven molecular motors

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Diphenylalanine peptide (FF) is well-known to form highly stable β -amyloid fibers. The difficulty to disrupt these aggregates is associated with numerous pathologies such as Alzheimer's disease.¹ The mechanical work produced by the rotation of artificial molecular motors has already been amplified in our group to influence the macroscopic properties of soft materials.^{2,3} In this work, we incorporated light-driven artificial molecular motors in carboxybenzyl-protected-FF (Z-FF) supramolecular hydrogels that form β -amyloid-like fibers. Interestingly, the mechanical work generated during the constant rotation of the molecular motor under UV light is sufficient to disrupt the β -amyloid fibers. This disruption was visible macroscopically as a gel-to-sol transition. In the absence of light, the system fully recovers its original microstructure. This unique reversible gel-sol transition phenomenon was studied by several techniques (rheology, TEM, AFM, CD, and SAXS) proving that the disruption of the β -amyloid fibers originates solely from the work generated by the out-of-equilibrium rotation of the molecular motor.⁴ These results highlight the potential of molecular motors to generate nanoscale mechanical work that targets biologically relevant structures, with expected applications in nanotechnologies and nanomedicine.

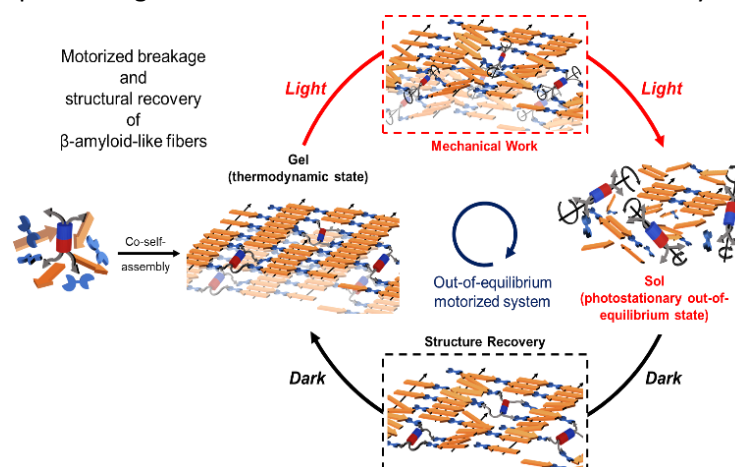


Figure 1. Schematic representation of the out-of-equilibrium motorized system based on supramolecular hydrogels.⁴

Acknowledgements.

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¹ J. D. Harper, P. T. Lansbury, *Annu. Rev. Biochem.* **1997**, *66*, 385–407

² Q. Li, G. Fuks, E. Moulin, M. Maaloum, M. Rawiso, I. Kulic, J. T. Foy, N. Giuseppone, *Nat. Nanotechnol.* **2015**, *10*, 161–165.

³ J. T. Foy, Q. Li, A. Goujon, J.-R. Colard-Itté, G. Fuks, E. Moulin, O. Schiffmann, D. Dattler, D. P. Funeriu, N. Giuseppone, *Nat. Nanotechnol.* **2017**, *12*, 540–545.

⁴ D. Daou, Y. Zarate, M. Maaloum, D. Collin, G. Fleith, D. Constantin, E. Moulin, N. Giuseppone, *Adv. Mater.* **2024**, *36*, 2311293.

Design, Synthesis and Physicochemical Properties of Nitrogen Modified Cryptophane A

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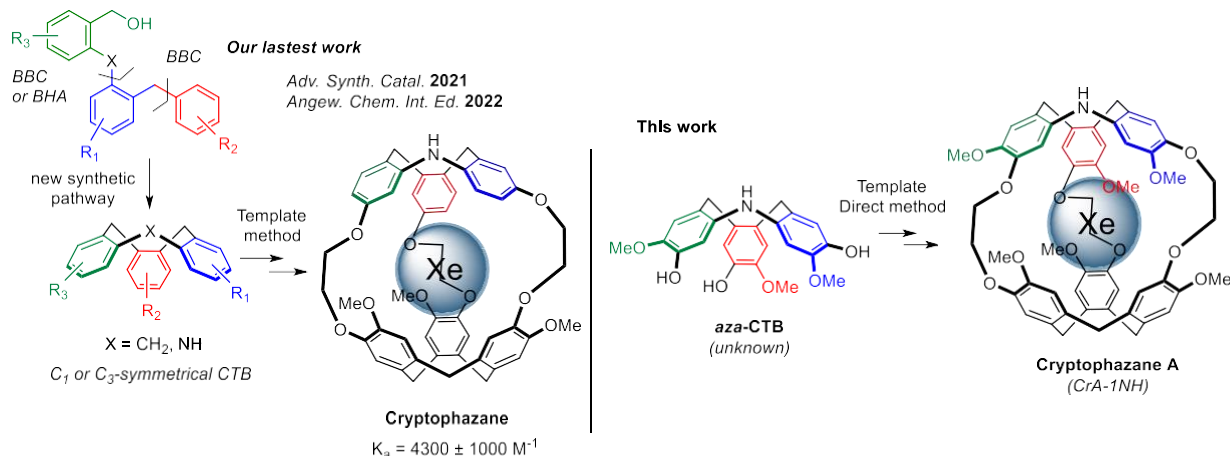
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Cryptophanes first synthesized by Collet in the early 1980s stand out due to their cage-like molecular architecture, consisting of two cyclotribenzylidene (CTB) units linked by three ether chains. This unique structure confers remarkable complexation properties with applications in chemistry, biology, and physics. Recently, particular interest has been shown as molecular probes for hyperpolarized xenon (HP ¹²⁹Xe) magnetic resonance imaging (MRI). However, the structural diversity of cryptophanes remains limited, largely due to the lack of versatile synthetic methodologies.

To address this challenge, our laboratory has developed a new polyfunctional approach enabling the controlled synthesis of CTBs with defined C₁ or C₃ symmetry.¹ Our project aims is to extend this strategy to access cryptophanes that have not been explored until now. This approach involves metal-free Barluenga-Boronic Coupling (BBC) for carbon-carbon bond formation, followed by palladium-catalyzed Buchwald-Hartwig Amination (BHA) to introduce heteroatom and final cyclization by electrophilic aromatic substitution (SEAr).

In this presentation, we will focus on the synthesis of an exact analogous of cryptophane A which could lead to unknown nitrogen modified cryptophane with improved properties for detection application as biosensor molecule in ¹²⁹Xe MRI. To achieve this, we will use our synthetic methodology and new functional groups will be introduced on the northern crown of cryptophazane. Finally, the host-guest properties of this cryptophane will be investigated using thermal ¹²⁹Xe NMR spectroscopy.



¹ (a) Vigier, C.; Fayolle, D.; El Siblani, H.; Sopkova - De Oliveira Santos, J.; Fabis, F.; Cailly, T.; Dubost, E. *Angew Chem Int Ed.* **2022**, *61* (46), e202208580. (b) Vigier, C.; Fossé, P.; Fabis, F.; Cailly, T.; Dubost, E. *Adv Synth Catal.* **2021**, *363* (15), 3756–3761.

Posters



Caged Macrocycles: Towards non-heme bioinspired catalysts

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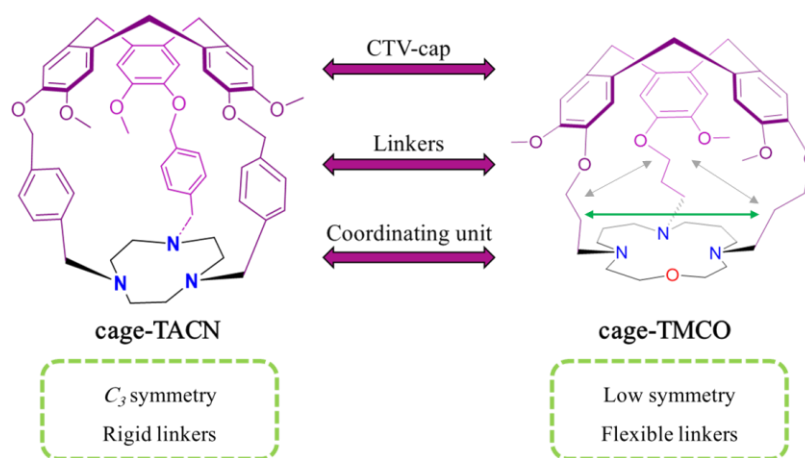
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Metalloenzymes are biocatalysts that catalyse difficult reactions with remarkable selectivity and efficiency. Cyclic polyamine ligands such as 1,4,7-triazacyclononane (**TACN**) and 1-oxa-4,8,12-triazacyclotetradecane (**TMCO**) are known for their ability to bind metal cations to form bioinspired catalysts.^[1,2] For instance, open Cu(I) **TACN**-based complexes can activate O₂ to produce powerful oxidizing species.^[3] Furthermore, Fe(II) **TMCO**-based complexes were used as model compounds for the study of oxygenases' mechanism.^[2]

However, in order to mimic metalloenzyme's activity, and improve the selectivity and efficiency of artificial catalysts, it is crucial to not only replicate the first coordination sphere, but also mimic the hydrophobic cavity surrounding the active site. To do so, it is possible to build supramolecular cages around artificial bioinspired complexes.

In particular, the cyclotrimeratrylene (**CTV**)-based hemicryptophane cage-ligands, have been used in our group enabling advanced catalysts and receptors (e.g., CH₄ oxidation).^[4] The goal of this work therefore is to reach unprecedented **TMCO** ligand and Cu(I)**TACN** complex equipped with hydrophobic cavities (Scheme 1). In particular, **cage-TMCO** displays a low symmetrical cavity offering 3 differently sized windows, getting closure to the low-symmetrical enzymatic cavities. Herein, the synthesis of two **TACN**- and one **TMCO**-based cages, displaying well-defined cavities of varying volumes and flexibility, is presented along with the study of their corresponding Cu(I) complexes as potential O₂ activating confined catalysts.



Scheme 1 Structure of the **TACN**-based caged (left) and structure of the **TMCO**-based caged ligand (right)

[5] R. Tripier, *et al. Inorg. Chem.* **2019**, 2669.

[6] K. Ray, *et al. Nat. Chem.* **2024**, 16 (4), 658–665.

[7] W. B. Tolman, *et al. Science* **1996**, 1397.

[8] (a) C. Colomban, *et al. Chem. Commun.* **2023**, 4288. (b) C. Colomban, *et al. JACS Au* **2024**, 1966

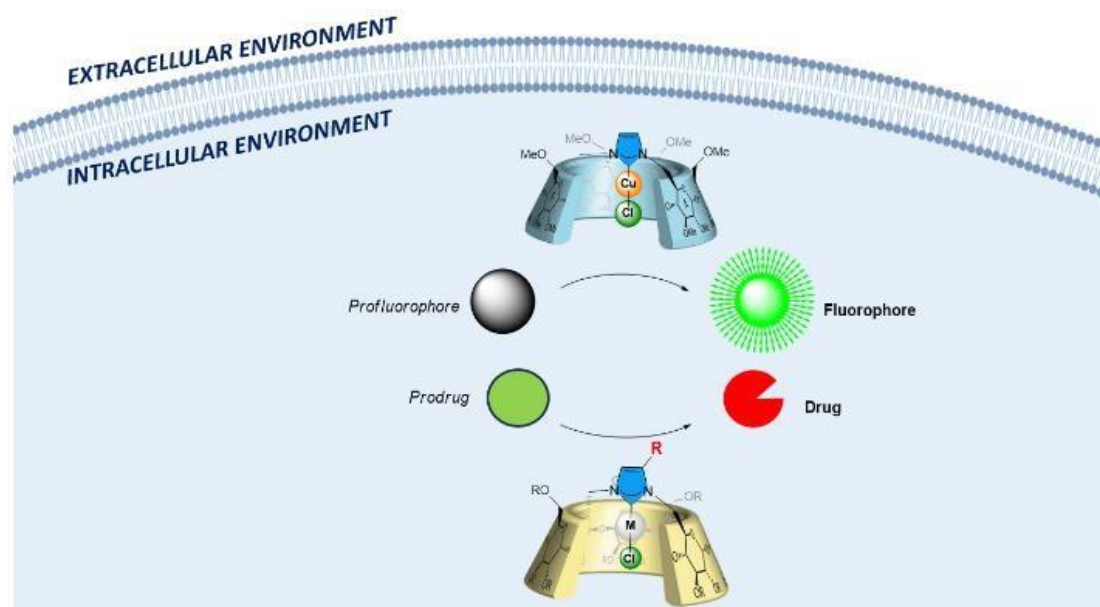
P2

Metal complexes based on modified cyclodextrins for the development of catalytic reactions in cells

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The use of organometallic catalysis in living cells offers promising avenues for imaging (via profluorophores) and therapeutic applications (via prodrugs). While most systems rely on rare and precious metals, copper(I) complexes represent an appealing alternative due to copper abundance and versatile reactivity.¹ However, intracellular copper catalysis face key challenges: metal toxicity, cellular uptake, competition with endogenous copper pools, stability, compatibility with complex cell media, and the need for biocompatible activation wavelengths in the case of photoactivation. Our group previously developed NHC-based metal complexes (Ag, Cu, Au, etc.),^{2,3,4} encapsulated in cyclodextrins (CDs), which protect the catalyst and preserve its catalytic activity while suppressing cytotoxicity. Building on this, we were able to carry out *ipso*-hydroxylation reactions of boronic esters in DMEM cell culture medium and in cancer cells, by using water-soluble NHC–copper complexes encapsulated in CDs, demonstrating their compatibility with complex biological environments. We now aim to adapt this system for cellular applications by improving cell permeability, enhancing intracellular copper competition, and by testing more stable NHC-based metal complexes—especially gold-based ones—to explore new orthogonal reactivities in cells.



- (5) Madec, H.; Figueiredo, F.; Cariou, K.; Roland, S.; Sollogoub, M.; Gasser, G. *Chem. Sci.* **2023**, *14*, 409–442.
- (6) Guitet, M.; Zhang, P.; Marcelo, F.; Tugny, C.; Jiménez-Barbero, J.; Buriez, O.; Amatore, C.; Mouriès-Mansuy, V.; Goddard, J.; Fensterbank, L.; Zhang, Y.; Roland, S.; Ménand, M.; Sollogoub, M. *Angew Chem Int Ed* **2013**, *52*, 7213–7218.
- (7) Zhang, P.; Meijide Suárez, J.; Driant, T.; Derat, E.; Zhang, Y.; Ménand, M.; Roland, S.; Sollogoub, M. *Angew. Chem Int Ed* **2017**, *129*, 10961–10965.
- (8) Zhu, X.; Xu, G.; Chamoreau, L.; Zhang, Y.; Mouriès-Mansuy, V.; Fensterbank, L.; Bistri-Aslanoff, O.; Roland, S.; Sollogoub, M. *Chem. Eur J* **2020**, *26* (68), 15901–15909.

Elaboration of non fullerene acceptors for Indoor Photovoltaics

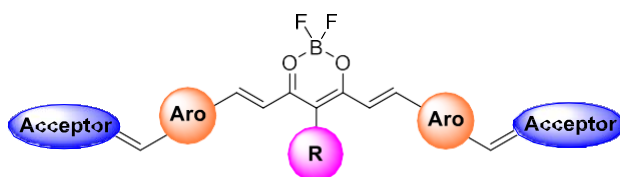
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Organic solar cells (OSCs) are light, flexible and easy to produce, with energy conversion efficiencies up to 19 %¹. However, they are not widely used for applications with artificial lighting, and their performance is limited, partly due to the use of fullerenes and their derivatives as electron acceptors in the active layer². To overcome these limitations, in this project, we are looking at curcuminoid derivatives to use them as non fullerene acceptors (NFAs). Curcumin is the main molecule of *Curcuma longa* L., also known as turmeric and has been used for centuries as a natural dye³ and for its medicinal properties⁴. These last decades, curcumin is also studied for its photophysical properties⁵ due to its 1,3-diketone core and its π -conjugated skeleton. Curcuminoid derivatives with a boron difluoride complex were synthesized to improve the curcumin photophysical properties⁶, and are mainly used as fluorescent tags, in optoelectronics⁷ like in OLEDs⁸, but also in OSCs. Archet *et al.*⁹ synthesized a curcuminoid derivative used as an electron donor in the active layer of OSCs, with power conversion energy up to 4.14 % and a high open-circuit voltage over 1.0 V, when associated with PC₆₁BM.

This project focuses on the development of a new family of NFAs: curcuminoid derivatives with a boron difluoride complex, whose structures are inspired by known NFAs. These compounds are synthesized and then characterized (UV-Vis absorbance, cyclic voltammetry, applications in OSCs).



General structure of curcuminoid derivatives as NFAs

¹ National Laboratory of the Rockies. *Best Research-Cell Efficiency Chart | Photovoltaic Research | NLR*.

² Xu, X.; Liu, W.; Luo, X.; Chen, H.; Wei, Q.; Yuan, J.; Zou, Y. *ChemSusChem* **2021**, *14* (17), 3428–3448.

³ Ravindran, P. N.; Babu, K. N.; Sivaraman, K. **2007**.

⁴ Lee, W.-H.; Loo, C.-Y.; Bebawy, M.; Luk, F.; Mason, R.; Rohanizadeh, R. *Curr. Neuropharmacol.* **2013**.

⁵ Benassi, R.; Ferrari, E.; Lazzari, S.; Spagnolo, F.; Saladini, M. *J. Mol. Struct.* **2008**, *892* (1–3), 168–176.

⁶ Ran, C.; Xu, X.; Raymond, S. B.; Ferrara, B. J.; Neal, K.; Bacskai, B. J.; Medarova, Z.; Moore, A. *J. Am. Chem. Soc.* **2009**, *131* (42), 15257–15261.

⁷ D'Aléo, A.; Zaborova, E.; Fagès, F. *Tech. Ing.* **2018**.

⁸ Gál, E.; Nagy, L. C.; Gál, E.; Nagy, L. C. *Symmetry* **2021**, *13* (12).

⁹ Archet, F.; Yao, D.; Chambon, S.; Abbas, M.; D'Aléo, A.; Canard, G.; Ponce-Vargas, M.; Zaborova, E.; Le Guennic, B.; Wantz, G.; Fages, F. *ACS Energy Lett.* **2017**, *2* (6), 1303–1307.

Porphyrin cages for photoredox catalysis of heterobiaryls

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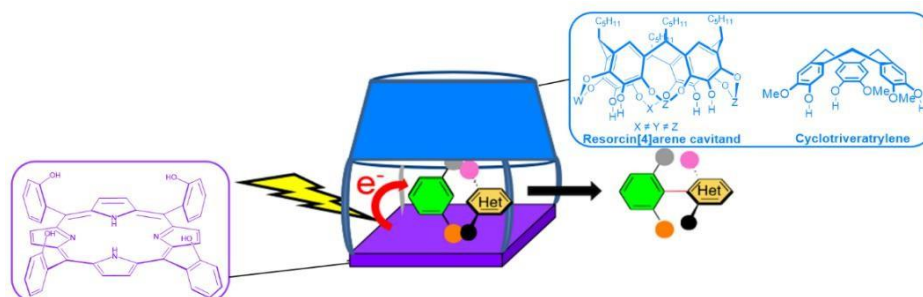
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Molecular cages are discrete compounds with cavities that can encapsulate smaller molecules through non-covalent interactions. They are designed for applications in molecular recognition, transport or catalysis. In supramolecular catalysis, they have demonstrated abilities to accelerate reactions, like Diels-Alder¹, and induce regio- and stereo-selectivity,² for example in the photodimerization of olefins.³ Recently, molecular cages with light-absorbing properties have emerged as promising systems for photocatalysis.^{4,5} However, metal-free covalent organic cages remain less explored than coordination cages, due to the need to integrate a photoactive unit.

In this project, new metal-free cages of different shapes and sizes are designed for supramolecular photoredox catalysis of enantioselective formation of heterobiaryls. These cages integrate a free-base porphyrin linked to a chiral concave capping unit: a cyclotrimeratrylene (CTV) or a resorcin[4]arene-based phosphonate cavitands (P-CAV). This design combines the photoredox activity of a porphyrin⁶ with the ability of the bowl-shaped component to stabilize encapsulated cations and neutral guests.⁷ Herein, we describe the synthesis of a CTV-porphyrin cage with triazole linkers by a templated approach and the preliminary results of the photoredox catalysis.



Porphyrin cages for the photoredox coupling of aryls diazonium salts and heteroarenes.

Acknowledgements. The ANR (ANR-23-CE07-0035 AtropoPhotoCat) and the GDR MAPYRO are gratefully acknowledged.

¹ M. Yoshizawa, M. Tamura, M. Fujita, *Science* **2006**, *312*, 251–254.

² M. Morimoto, S. M. Bierschenk, K. T. Xia, R. G. Bergman, K. N. Raymond, F. D. Toste, *Nat. Catal.* **2020**, *3*, 969–984.

³ M. Yoshizawa, Y. Takeyama, T. Kusakawa, M. Fujita, *Angew. Chem. Int. Ed.* **2002**, *41*, 1347–1349

⁴ R. Ham, C. J. Nielsen, S. Pullen, J. N. H. Reek, *Chem. Rev.* **2023**, *123*, 5225–5261.

⁵ S. Tanaka, T. Nakazono, K. Yamauchi, K. Sakai, *Chem. Lett.* **2017**, *46*, 1573–1575.

⁶ D. Gryko, K. Rybicka-Jasińska, B. König, *Eur. J. Org. Chem.* **2017**, *2017*, 2104–2107.

⁷ D. Zhang, A. Martinez, J.-P. Dutasta, *Chem. Rev.* **2017**, *117*, 4900–4942

Not going back: Unidirectional movement by intramolecular one-way ratcheting of functionalized cyclodextrin

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Molecular motion is vital for life, driving essential processes at the nanoscale within living cells. This is made possible by biomolecular motors, which can perform unidirectional motion. For example, kinesin motor proteins transport cargos along microtubules.¹ Such directional movement arises from biasing Brownian motion through chemically fueled Brownian ratcheting mechanisms.² Natural systems have inspired scientists to design artificial molecular motors.³ While unidirectional motion has been achieved using information ratchet mechanisms in rotaxanes and catenanes,^{4,5} exploiting the intrinsic asymmetry of a three-dimensional macrocycle to drive motion via ratcheting remains unexplored.

In this work, we present an information ratchet that exploits the inherent asymmetry of cyclodextrin's cone-shaped macrocycle to achieve directional motion in a rotaxane. By selectively functionalizing the cyclodextrin small rim, we enable a mechanospecific deprotection of temporary stoppers positioned on the rotaxane axle in front of the CD. As a result, under chemical fueling, the CD moves autonomously in a single direction by opening the stoppering gates exclusively one way, and subsequently favoring their closure⁶ once it has passed through. This system demonstrates a synergistic, double-gated, one-way ratchet mechanism driven by the unique asymmetrical structure of the cyclodextrin paving the way toward long-range linear molecular motors (Figure 1).⁷

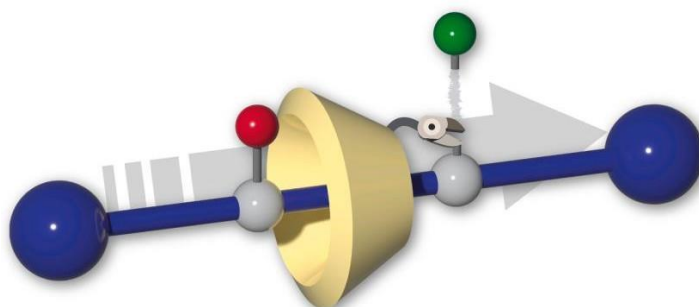


Figure 1. Schematic representation of the double-gated one-way ratcheted system.⁷

¹N. Hirokawa, Y. Noda, Y. Tanaka, S. Niwa, *Nat. Rev. Mol. Cell Biol.* **2009**, *10*, 682–696.

²M. Schliwa, G. Woehlke, *Nature* **2003**, *422*, 759–765.

³S. Erbas-Cakmak, D. A. Leigh, C. T. McTernan, A. L. Nussbaumer, *Chem. Rev.* **2015**, *115*, 10081–10206.

⁴Y. Ren, R. Jamagne, D. J. Tetlow, D. A. Leigh, *Nature* **2022**, *612*, 78–82.

⁵M. R. Wilson, J. Solà, A. Carlone, S. M. Goldup, N. Lebrasseur, D. A. Leigh, *Nature* **2016**, *534*, 235–240.

⁶E. Liu, S. Cherraben, L. Boulo, C. Troufflard, B. Hasenknopf, G. Vives, M. Sollogoub, *Chem* **2023**, *9*, 1147–1163.

⁷E. Liu, D. Daou, B. Hasenknopf, G. Vives, M. Sollogoub, *Chem* **2025**, 102623.

Low-Symmetry Hemicryptophanes functionalized with Azaphosphatrane derivatives

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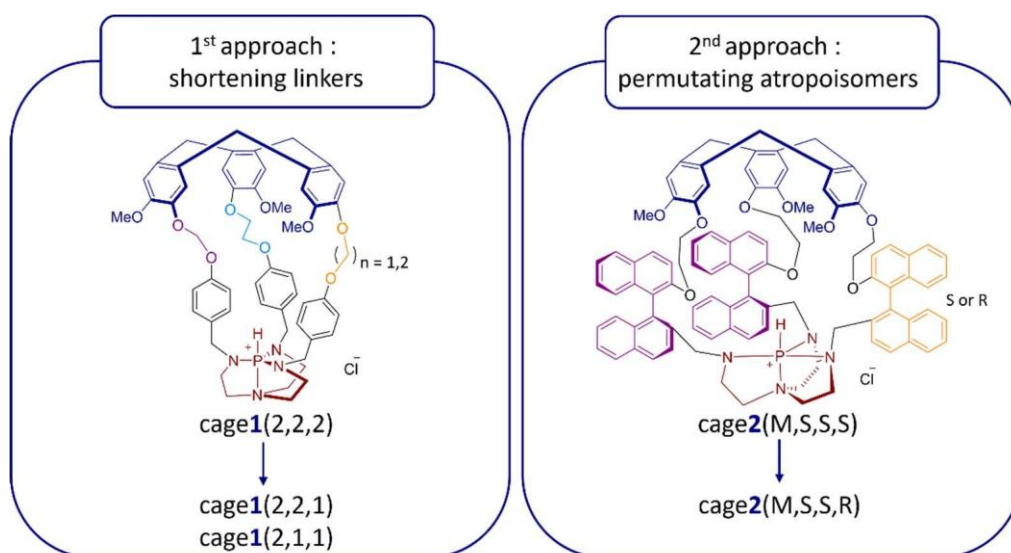
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Azaphosphatranes (in red in Scheme below) are pro-azaphosphatrane's acidic counterparts, stable species that could be used to generate reactive **pro-azaphosphatranes** in a single step.¹ The latter, also known as Verkade's superbases, were discovered in 1989 by Verkade. These species are highly basic with a pKa around 32 in CH₃CN. Pro-azaphosphatranes have been used as basic and nucleophilic catalysts in various transformations, such as isocyanurate formation or Strecker reaction.²

Previously in the team³, we reported an endohedral functionalized cage displaying catalytic activity in **base-catalysed Diels-Alder reaction** between prochiral 3-hydroxy-2-pyrone and various dienophiles through activation with encaged pro-azaphosphatrane as base. The crucial role of the molecular cavity on catalytic performance was highlighted.

On this basis, the objective is to access **low-symmetry endohedral cages** (Scheme below) using two innovative methods, thus enabling better substrate selectivity and diastereoselectivity. One aspect of this work deals with the tuning of linkers' length to functionalize the azaphosphatrane moiety with the enantiopure **CTV cap** (Scheme, left). Another approach uses three enantiopure 1,1'-binaphthyl linkers, creating a highly chiral hemicryptophane cage 2 (Scheme, right) for enantioselective catalysis. Cage syntheses will be presented with the study of corresponding pro-azaphosphatrane bases as catalysts.



Acknowledgements. This project has been carried out with the financial support of the A*MIDEX (no. AMX-22-RE-AB-141), funded by the Investissements d'Avenir project of the French Government (ANR).

¹ B. A. D'S, J. G. Verkade, *J. Org. Chem.* **1996**, 61 (9), 2963–2966

² J. G. Verkade, P. B. Kisanga, *Tetrahedron* **2003**, 59 (40), 7819–7858

³ Chatelet, B., Dufaud, V., Dutasta, J.-P. & Martinez, A. *J. Org. Chem.* **2014**, 79 (18), 8684–8688

Ordered Honeycomb Host–Guest Networks on HOPG for Supported Asymmetric Catalysis

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Although heterogeneous catalysis offers clear advantages in terms of catalyst recovery and reuse, achieving high efficiency and cooperative effects between catalytic units remains difficult, especially for asymmetric transformations. Here, we aim to develop an ordered catalytic platform for the asymmetric hydrolysis of small meso-epoxides using salen complexes.

Our approach relies on the self-assembly of 3,5-Tri-(*E*)-styrylbenzene (TSB) on graphene to form a two-dimensional honeycomb-like molecular sieve¹. This supramolecular monolayer generates regular pores capable of accommodating polyaromatic species through non-covalent interactions². We propose to exploit this host–guest architecture to position pyrene-functionalized salen catalysts³ within the pores, thereby controlling their spatial arrangement at the surface. By tuning the inter-catalyst distance, we seek to reproduce the cooperative behavior previously observed between paired salen units⁴, with the goal of enhancing both enantioselectivity and reaction kinetics.

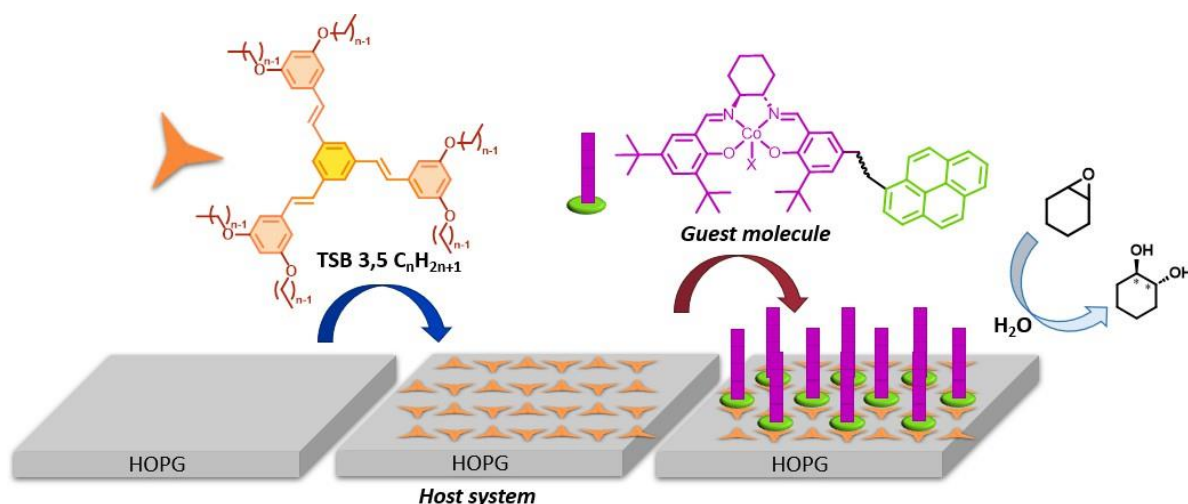


Figure 1. Hosting of pyrene-tagged Co-salen catalyst into the pores of the honeycomb system formed by the self assembly of TSB on graphene

¹ Bléger, D.; Kreher, D.; Mathevet, F.; Attias, A.-J.; Schull, G.; Huard, A.; Douillard, L.; Fiorini-Debuischert, C.; Charra, F. *Surface, Angew. Chem. Int. Ed.* **2007**, *46* (39), 7404–7407

² Schull, G.; Douillard, L.; Fiorini-Debuischert, C.; Charra, F.; Mathevet, F.; Kreher, D.; Attias, A.-J., *Adv. Mater.* **2006**, *18* (22), 2954–2957

³ Abd El Sater, M.; Mellah, M.; Dragoie, D.; Kolodziej, E.; Jaber, N.; Schulz, E., *Chem. – Eur. J.* **2021**, *27* (36), 9454–9460

⁴ Ready, J. M.; Jacobsen, E. N., *J. Am. Chem. Soc.* **2001**, *123* (11), 2687–2688

Chiroptical bis-(acridinium-Zn(II)porphyrin) Tweezers

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Porphyrins are known as excellent chromophores and fluorophores whose optical properties can be tuned by metal coordination.¹ These features make metalloporphyrins highly attractive for the chiroptical detection of non-absorbing chiral coordinating substrates. In particular, the close spatial arrangement of two porphyrin units can lead to a pronounced exciton coupling in the visible range.² Our group has explored the pH switching of acridinium units coupled to porphyrins in a tweezer architecture, and has recently demonstrated the possibility of switching the porphyrin luminescence in an on/off manner.³ We are now focusing on developing novel switchable acridinium-metalloporphyrin systems to investigate the chiroptical detection of substrates upon commutation, using both exciton-coupled circular dichroism (ECCD) and circularly polarized luminescence (CPL).⁴ In this context, we have synthesized two different bis-(acridinium-Zn(II)porphyrin) tweezers, which enable sensitive and intense chiroptical detection in the visible range (Figure 1).

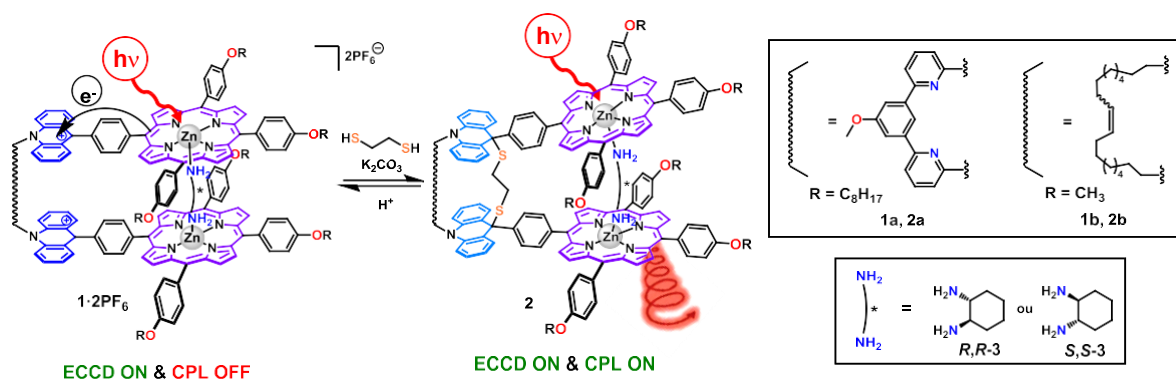


Figure 1. Chiral diamine recognition by a bis-(acridinium-Zn(II)porphyrin) tweezer and his luminescence switching properties

Acknowledgements. We would like to thank the University of Strasbourg, the CNRS, and the ENS Paris-Saclay for their financial support. This work was supported by the Interdisciplinary Thematic Institute SysChem via the IdEx Unistra (ANR-10-IDEX-0002) within the program Investissement d'Avenir ».

¹ A. R. Sekhar, Y. Chitose, J. Janoš, S. I. Dangoor, A. Ramundo, R. Satchi-Fainaro, P. Slaviček, P. Klán, R. Weinstain, *Nat. Commun.* **2022**, *13* (1), 3614.

² X. Huang, B. H. Rickman, B. Borhan, N. Berova, K. Nakanishi, *J. Am. Chem. Soc.* **1998**, *120* (24), 6185–6186.

³ 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* (19), 10691–10699.

⁴ K. Dhbaibi, P. Matozzo, L. Abella, M. Jean, N. Vanthuyne, J. Autschbach, L. Favereau, J. Crassous, *Chem. Commun.* **2021**, *57* (82), 10743–10746.

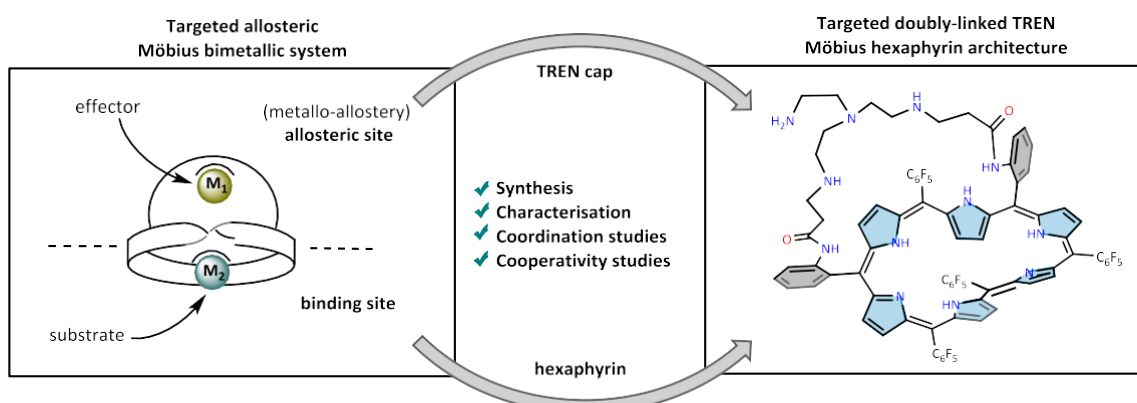
Möbius hexaphyrins with an overhanging metal binding site as unprecedented allosteric receptors

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Biomimicking has always been of great interest for decades. Nature shows remarkable specificity in metal involved biochemical processes through properties like allostery. Allostery involves the conformational change caused due to the effect on the allosteric site which in turn affects the affinity of the binding site. This specific property has been ubiquitous in enzymes and receptors.¹ To attain this kind of specificity, expanded porphyrins would be suitable platforms due to their fascinating properties such as topology, π -conjugation, coordination behaviour, aromaticity and reactivity.² The engineering of molecular receptors based on expanded porphyrins is quite under explored and challenging. From the previous work in our group, an hexaphyrin with a triply-linked TREN [tris(2-aminoethyl) amine] cap was proved to be a molecular host with a confined space accommodating a metal at the level of the Möbius hexaphyrin N-core, thereby enabling the binding of two guest molecules.³ In this work, we have improved our design and synthesized a Möbius hexaphyrin which is doubly-linked to the TREN cap. A free amino arm enables the metal coordination both at the level of the hexaphyrin as well as in the TREN, giving a bimetallic Zn (II) complex. The coordination of the metal at the level of TREN modifies the binding environment at the hexaphyrin N-core for the guest molecules (Hückel antiaromatic to Möbius aromatic conversion). This unique behaviour exhibited by the complex makes it an appropriate candidate for the further studies of allostery in Möbius type-receptors. To our knowledge, this is the very first example of a Möbius ring with an overhanging metal binding site.



Acknowledgements. The University of Rennes is acknowledged for the financial support.

¹ Kovbasyuk, L. & Krämer, R. Allosteric Supramolecular Receptors and Catalysts. *Chem. Rev.* **104**, 3161–3188 (2004).

² Tanaka, T. & Osuka, A. Chemistry of meso -Aryl-Substituted Expanded Porphyrins: Aromaticity and Molecular Twist. *Chem. Rev.* **117**, 2584–2640 (2017).

³ Ruffin, H. *et al.* Tren-Capped Hexaphyrin Zinc Complexes: Interplaying Molecular Recognition, Möbius Aromaticity, and Chirality. *J. Am. Chem. Soc.* **139**, 13847–13857 (2017).

Insights into self-assembly mechanisms and electrical properties of tetrazine-based supramolecular polymers

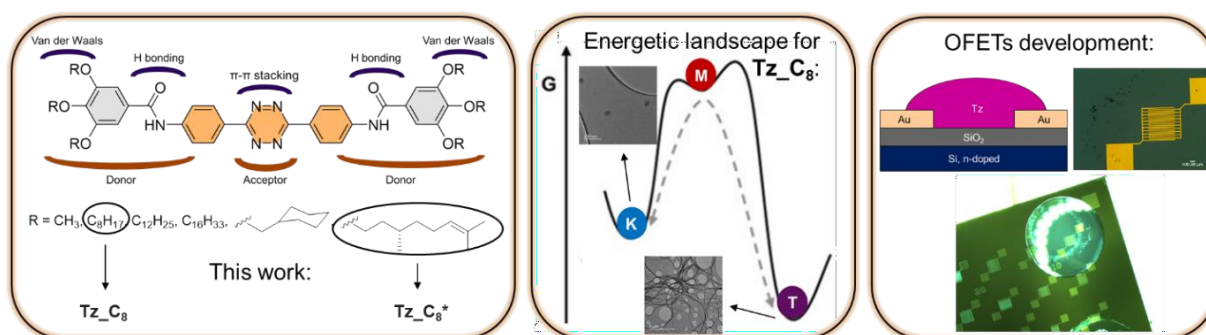
Lucrezia Trevisan,^[a,b] William T. Gallonde,^[a] Zuchong Yang,^[b] Vincent Dorcet,^[a] Arnaud Saint-Jalmes,^[c] Emanuele Orgiu,^[b] Stéphane Rigaut,^[a] Olivier Galangau*^[a]

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Supramolecular polymers are composed of monomeric units held together by highly directional and reversible secondary non-covalent interactions, resulting in dynamic species that can exhibit properties such as self-healing functions and responsiveness towards external stimuli.¹ Originally, supramolecular polymerization was regarded as a process entirely driven by thermodynamics. However, as the understanding of this process broadened, kinetic contributions started to emerge as impactful factors towards the outcome of the self-assembly, and multiple pathways in competition for the same monomer can occur. In particular, experimental conditions (*e.g.*, temperature or solvent modulation) and specific interactions (*e.g.*, donor-acceptor interactions) can have significant impact on the polymerization.^{2,3} We recently developed a new family of supramolecular polymers, featuring a central tetrazine core and different aliphatic side chains, resulting in donor-acceptor-donor structures with interesting self-assembly mechanisms. In determined conditions, supramolecular gels can be obtained, and given the electron properties (*e.g.*, available reduction potentials, electron deficiency) exhibited by tetrazine, these materials can be studied towards the development of novel n-type organic semiconductors.⁴ In this work, the self-assembly of two of these platforms (**Tz_C₈** and **Tz_C₈***) is explored, describing how subtle structural differences can not only impact the morphologies of these systems, but also their evolution towards thermodynamic equilibrium. Additionally, preliminary studies on their conductive capabilities are reported, with the development of organic field effect transistors (OFETs) featuring the tetrazine-based supramolecular gels.



¹ T. F. A. De Greef et al., *Chem. Rev.* **2009**, *109*, 5687–5754.

² J. Matern et al., *Angew. Chem. Int. Ed.* **2019**, *58*, 16730 – 16740.

³ F. Wang et al., *Angew. Chem. Int. Ed.* **2023**, *62*, e202305827.

⁴ G. Clavier, P. Audebert, *Chem. Rev.* **2010**, *110*, 3299–3314.

Mechanical disruption of β -Amyloid fiber analogs by out-of-equilibrium operation of light-driven molecular motors

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Diphenylalanine peptide (FF) is well-known to form highly stable β -amyloid fibers. The difficulty to disrupt these aggregates is associated with numerous pathologies such as Alzheimer's disease.¹ The mechanical work produced by the rotation of artificial molecular motors has already been amplified in our group to influence the macroscopic properties of soft materials.^{2,3} In this work, we incorporated light-driven artificial molecular motors in carboxybenzyl-protected-FF (Z-FF) supramolecular hydrogels that form β -amyloid-like fibers. Interestingly, the mechanical work generated during the constant rotation of the molecular motor under UV light is sufficient to disrupt the β -amyloid fibers. This disruption was visible macroscopically as a gel-to-sol transition. In the absence of light, the system fully recovers its original microstructure. This unique reversible gel-sol transition phenomenon was studied by several techniques (rheology, TEM, AFM, CD, and SAXS) proving that the disruption of the β -amyloid fibers originates solely from the work generated by the out-of-equilibrium rotation of the molecular motor.⁴ These results highlight the potential of molecular motors to generate nanoscale mechanical work that targets biologically relevant structures, with expected applications in nanotechnologies and nanomedicine.

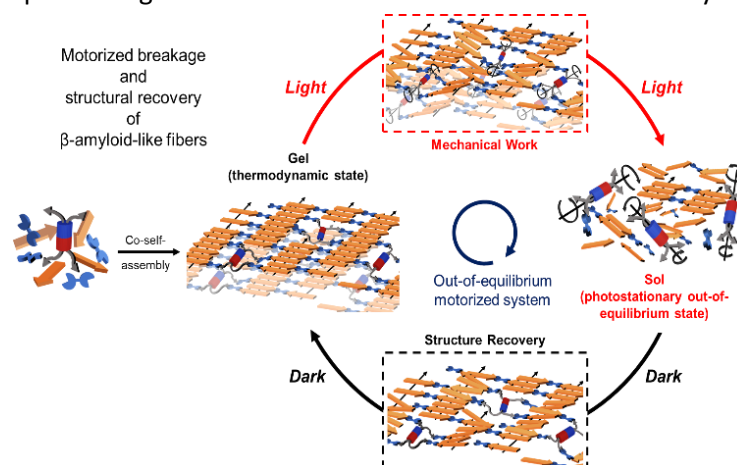


Figure 1. Schematic representation of the out-of-equilibrium motorized system based on supramolecular hydrogels.⁴

Acknowledgements.

This work was granted by the European Commission's Horizon 2020 Program as part of the MSCA-ITN project ArtMoMa under grant no. 860434.

¹ J. D. Harper, P. T. Lansbury, *Annu. Rev. Biochem.* **1997**, *66*, 385–407

² Q. Li, G. Fuks, E. Moulin, M. Maaloum, M. Rawiso, I. Kulic, J. T. Foy, N. Giuseppone, *Nat. Nanotechnol.* **2015**, *10*, 161–165.

³ J. T. Foy, Q. Li, A. Goujon, J.-R. Colard-Itté, G. Fuks, E. Moulin, O. Schiffmann, D. Dattler, D. P. Funeriu, N. Giuseppone, *Nat. Nanotechnol.* **2017**, *12*, 540–545.

⁴ D. Daou, Y. Zarate, M. Maaloum, D. Collin, G. Fleith, D. Constantin, E. Moulin, N. Giuseppone, *Adv. Mater.* **2024**, *36*, 2311293.

Design, Synthesis and Physicochemical Properties of Nitrogen Modified Cryptophane A

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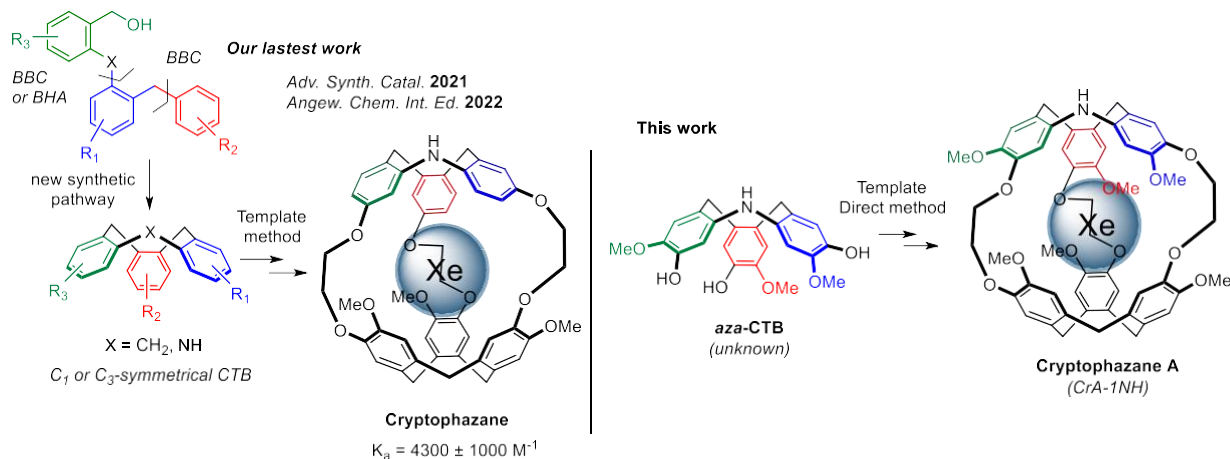
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Cryptophanes first synthesized by Collet in the early 1980s stand out due to their cage-like molecular architecture, consisting of two cyclotribenzylidene (CTB) units linked by three ether chains. This unique structure confers remarkable complexation properties with applications in chemistry, biology, and physics. Recently, particular interest has been shown as molecular probes for hyperpolarized xenon (HP ¹²⁹Xe) magnetic resonance imaging (MRI). However, the structural diversity of cryptophanes remains limited, largely due to the lack of versatile synthetic methodologies.

To address this challenge, our laboratory has developed a new polyfunctional approach enabling the controlled synthesis of CTBs with defined C₁ or C₃ symmetry.¹ Our project aims is to extend this strategy to access cryptophanes that have not been explored until now. This approach involves metal-free Barluenga-Boronic Coupling (BBC) for carbon-carbon bond formation, followed by palladium-catalyzed Buchwald-Hartwig Amination (BHA) to introduce heteroatom and final cyclization by electrophilic aromatic substitution (S_EAr).

In this presentation, we will focus on the synthesis of an exact analogous of cryptophane A which could lead to unknown nitrogen modified cryptophane with improved properties for detection application as biosensor molecule in ¹²⁹Xe MRI. To achieve this, we will use our synthetic methodology and new functional groups will be introduced on the northern crown of cryptophazane. Finally, the host-guest properties of this cryptophane will be investigated using thermal ¹²⁹Xe NMR spectroscopy.



¹ (a) Vigier, C.; Fayolle, D.; El Siblani, H.; Sopkova - De Oliveira Santos, J.; Fabis, F.; Cailly, T.; Dubost, E. *Angew Chem Int Ed.* **2022**, *61* (46), e202208580. (b) Vigier, C.; Fossé, P.; Fabis, F.; Cailly, T.; Dubost, E. *Adv Synth Catal.* **2021**, *363* (15), 3756–3761.

Molecular Porous Host•Guest Crystals

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Recently, porous organic crystals (**POC**) based on macrocycles have shown exceptional sorption and separation properties.¹ Yet, the impact of guest presence inside a macrocycle prior to crystallization and adsorption has not been studied. We will show that the inclusion of trimethoxybenzyl-azaphosphatrane in the macrocycle cucurbit[8]uril (CB[8]) affords molecular porous host•guest crystals (**PHGC**) with radically new properties.² Not only the guest could tune the porous space of CB[8] crystals, but also unactivated hydrated **PHGC** could adsorb iodine spontaneously and selectively at room temperature and atmospheric pressure. The absence of (i) heat for material synthesis, (ii) moisture sensitivity, and (iii) energy-intensive steps for pore activation are attractive attributes to produce porous materials at low energetic costs. ¹H NMR and DOSY were instrumental for monitoring the H₂O/I₂ exchange and iodine-doped crystals showed markedly different second harmonic generation (SHG).

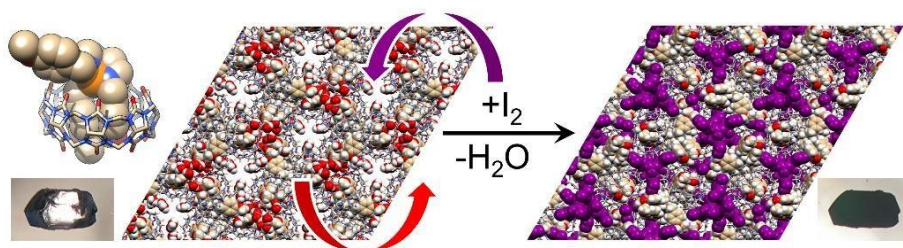


Figure 1. Host•guest complex with CB[8], packing showing 1D channels and iodine adsorption.

Acknowledgements. CNRS and Aix Marseille Université are acknowledged for continuous support. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 713750. Also, it has been carried out with the financial support of the Regional Council of Provence-Alpes-Côte d'Azur and with the financial support of the A*MIDEX (no. ANR-11- IDEX-0001-02), funded by the Investissements d'Avenir project of the French Government (ANR).

¹ H. Zhu, L. Chen, B. Sun, M. Wang, H. Li, J. F. Stoddart, F. Huang, *Nat. Rev. Chem.* **2023**, *7*, 768-782.

² X. Yang, C. Li, M. Giorgi, D. Siri, X. Bugaut, B. Chatelet, D. Gigmes, M. Yemloul, V. Hornebecq, A. Kermagoret, S. Brasselet, A. Martinez, D. Bardelang, *Angew. Chem. Int. Ed.* **2022**, *61*, e202214039.

If You Seek ^{11}B : Confining a Boranylium Cation in the Cavity of Cyclodextrins

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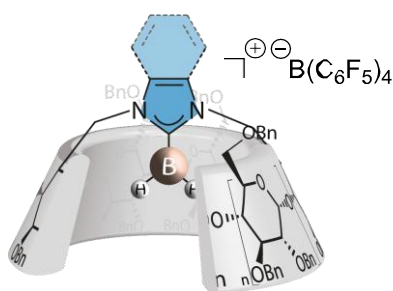
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Cyclodextrins (CDs) have been studied as platforms for selective catalytic reactions. The bridging of CDs with *N*-heterocyclic carbene (NHC) ligands allowed the formation of diverse metallic complexes confined inside the cavity. Reactions involving coinage metals (Cu, Ag, Au) have been described and showed great regio-, enantio- and even substrate-selectivities towards hydroboration, cycloisomerization and alkoxy cyclization reactions.¹

We recently turned our interest towards the confinement of organocatalysts to study the influence of the cavity in metal-free reactions.

NHC-borenylium cations have been studied during the past years for their strong Lewis acidity allowing the activation of H_2 and of CH_4 .² While many modifications were brought to the structure of the cations, none were confined in discrete cavities.

We therefore synthesized NHC-BH₃ boranes confined in the cavity of CDs. The presence of the cavity led to a drastic, unpredicted, decrease in the relaxation time of the boron nucleus in NMR. The corresponding cation was formed by hydride abstraction and its ^{11}B signal only observable using a 1 GHz NMR spectrometer. Its Lewis acidity and reactivity were subsequently studied and proved the obtention of the first cavity-confined Lewis superacid.



Boranes confined within the α -, β - & γ -CD

Boranylium cations:

First confined Lewis Superacids

¹ a) P. Zhang, C. Tugny, J. Meijide Suárez, M. Guitet, E. Derat, N. Vanthuyne, Y. Zhang, O. Bistri, V. Mouriès-Mansuy, S. Roland, L. Fensterbank, M. Sollogoub, *Chem* **2017**, *3*, 174; b) S. Roland, J. Meijide Suárez, M. Sollogoub, *Chem. Eur. J.* **2018**, *24*, 12464; c) C. Tugny, N. del Rio, M. Koohgard, N. Vanthuyne, D. Lesage, K. Bijouard, P. Zhang, J. Meijide Suárez, S. Roland, E. Derat, O. Bistri-Aslanoff, M. Sollogoub, L. Fensterbank, V. Mouriès-Mansuy, *ACS Catal.* **2020**, *10*, 5964.

² a) J. Farrell, J. Hatnean, D. Stephan, *J. Am. Chem. Soc.* **2012**, *134*, 15728; b) Y. Liu, W. Dong, Z. H. Li, H. Wang, *Chem* **2021**, *7*, 1843.

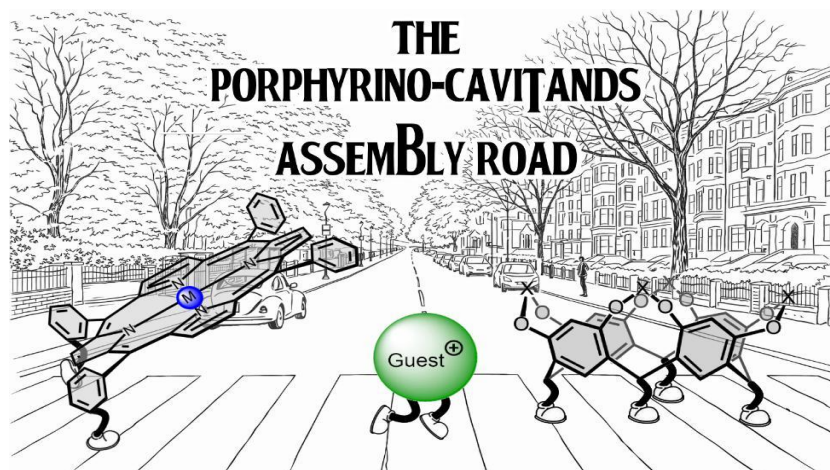
The Porphyrino-cavitands: synthesis and supramolecular assemblies

Kajetan Bijouard,^[a] **Sandrine Denis-Quanquin**,^[a] **Jean-Christophe Mulatier**,^[a] **Delphine Pitrat**,^[a] **Louise Pfeiffer**,^[b]
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Inspired by Nature's ability to perform specific and selective reactions using enzymes, chemists have sought to confine catalytic centers in artificial pockets. One strategy aims at using covalent molecular cages. To this end, catalytic centers have been successfully confined in cyclodextrins, calixarenes, cyclophanes and many others.¹ Among them, calix[4]resorcinarene-based cavitands have been studied for decades, mainly for their host-guest properties.² These cages can be functionalized, creating deeper cavities suitable for confined catalysis.² For this project, the cavitand was decorated with porphyrins which are well known for their catalytic abilities.^{3,4} As part of this study, we studied the supramolecular assemblies of the two parent macrocycles with different guests to assess the molecular cages' capabilities to confine different reactants.



Acknowledgements. The authors acknowledge the French National Research Agency for financial support (ANR-23-CE07-0035 AtropoPhotoCat).

¹ a) S. Roland, J. Mejjide Suárez, M. Sollogoub, *Chem. Eur. J.* **2018**, *24*, 12464; b) K. Bijouard, E. Nicolas, L. Anthore-Dalio, M. Sollogoub, T. Cantat, *Chem. Eur. J.* **2025**, *31*, e202403955; c) L. Le Clainche, Y. Rondelez, O. Sénèque, S. Blanchard, M. Campion, M. Giorgi, A. Duprat, Y. Le Mest, O. Renaud, *Comptes Rendus Académie Sci. - Ser. IIC - Chem.* **2000**, *3*, 811; d) R. Roy, A. Kar, S. Paul, S. Mohapatra, S. Gosh, *J. Org. Chem.* **2023**, *88*, 14388.

² a) V. Jain, P. Kanaiya, *Russ. Chem. Rev.* **2011**, *80*, 75; b) N. Natarajan, E. Brenner, D. Sémeril, D. Matt, J. Harrowfield, *Eur. J. Org. Chem.* **2017**, *41*, 6100; c) P. Delangle, J.-C. Mulatier, B. Tinant, J.-P. Declercq, J.-P. Dutasta, *Eur. J. Org. Chem.* **2001**, *19*, 3695.

³ L. Schoepff, L. Monnereau, S. Durot, S. Jenni, C. Gourlaouen, V. Heitz, *ChemCatChem* **2020**, *12*, 5826.

⁴ M. McKay, T. Cwele, H. Friedrich, G. Maguire, *Org. Biomol. Chem.* **2009**, *7*, 3958.

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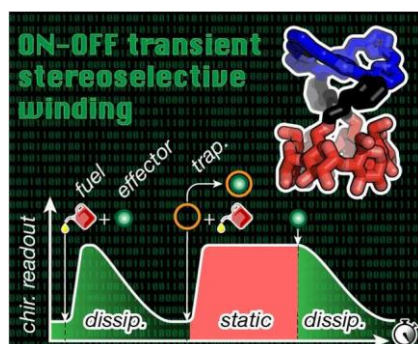
Time-Programmable Chiroptical Response from a Möbius Totemic Architecture

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The transient stereoselective winding of a Möbius aromatic π -system has been achieved for the first time, affording a dynamic and tunable chiroptical response in the time domain. This system results from the synergistic action of i) a totemic chiral edifice (hexaphyrin-cyclodextrin hybrid), ii) a carboxylic acid fuel (trichloroacetic acid), iii) an exchange of counterion with Cl⁻, allowing the dissipative process to be turned on and off.¹



Acknowledgements. We are grateful to the Agence Nationale de la Recherche for financial support (ANR-20-CE07-0026).

¹ S. Dash, M. Ménand, S. Le Gac, *ChemistryEurope* **2026**, 4, e202500466.

Light-Frozen Dynamic Covalent Synthesis of Extended Diimide-incorporating Macrocycles

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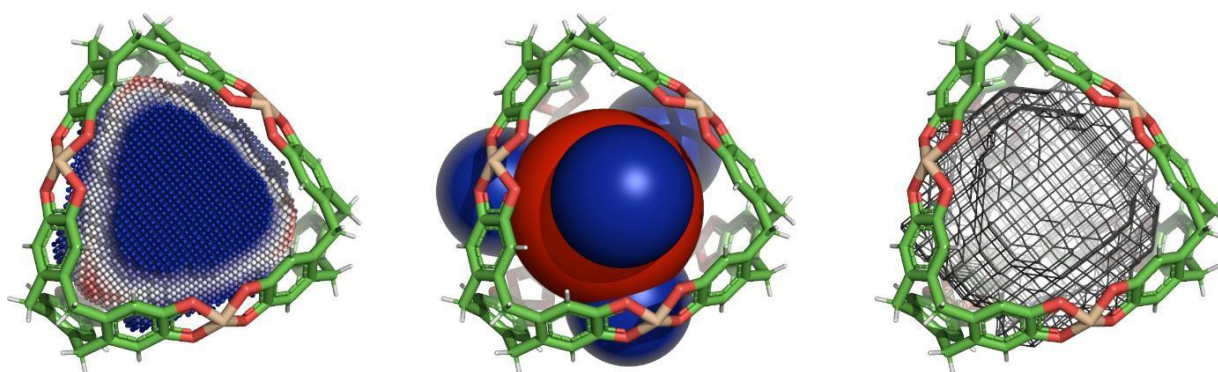
In recent years, conjugated macrocycles have gained significant interest due to their unique properties. Unlike their linear counterparts, they feature a well-defined internal cavity capable of accommodating host molecules and show enhanced charge delocalization throughout the cyclic structure.¹ Among these systems, cycloparaphenylenes (CPPs) are especially notable for their optical and electronic properties.² However, their synthesis remains challenging, involving multiple steps, low overall yields, and the use of precious-metal-based reagents. Consequently, structural diversification is time-demanding, and only a few electron-deficient derivatives have been reported.^{3,4} Notably, perylene diimide (PDI)-based macrocycles introduced by C. Nuckolls have been successfully used as n-type semiconductors for electron transport in solar cells and organic photodetectors.⁵ F. Würthner and co-workers have extensively studied Coronene Diimide (CDI)-based cyclophanes, emphasizing their strong host-guest interactions, which enable the encapsulation of large π -conjugated guests via π - π and C-H- π interactions.⁶ T. Barendt and collaborators reported the synthesis of flexible cyclophanes based on PDI units and demonstrated solvent-dependent switching of their chiroptical properties.⁷

This work focuses on studying new π -extended cyclophanes using a novel synthesis method based on dynamic covalent chemistry. The targeted macrocycles will be prepared through the condensation of flexible or rigid bisaldehydes with 1,6- or 1,7-diamino perylene diimide PDI-(NH₂)₂.⁸ Their size will be controlled by adjusting the reaction conditions, templates, and the geometry, size, and rigidity of the aldehyde precursors. Visible-light will be employed to freeze the system. The resulting macrocycles will then be investigated for their optoelectronic and host-guest properties.

- (1) Iyoda, M.; Yamakawa, J.; Rahman, M. J. *Angew. Chem. Int. Ed.* **2011**, *50* (45), 10522–10553.
- (2) Leonhardt, E. J.; Jasti, R. *Nat. Rev. Chem.* **2019**, *3* (12), 672–686.
- (3) Lewis, S. E. *Chem. Soc. Rev.* **2015**, *44* (8), 2221–2304.
- (4) Hermann, M.; Wassy, D.; Esser, B. *Angew. Chem. Int. Ed.* **2021**, *60* (29), 15743–15766.
- (5) Ball, M.; Zhang, B.; Zhong, Y.; Nuckolls, C. *Acc. Chem. Res.* **2019**, *52* (4), 1068–1078.
- (6) Garain, S.; Würthner, F. *Chem. Commun.* **2025**, *61* (15), 3081–3092.
- (7) Hartmann, D.; Penty, S. E.; Zwijnenburg, M. A.; Pal, R.; Barendt, T. A. *Angew. Chem. Int. Ed.* **2025**, *64* (15), e202501122.
- (8) Goujon, A.; Rocard, L.; Cauchy, T.; Hudhomme, P. *J. Org. Chem.* **2020**, *85* (11), 7218–7224.

pyKVFinder: A new cavity characterization software for supramolecular cagesJoão V. S. Guerra,^[a] Luiz F. G. Alves^[a], Didier Bourissou,^[b] Paulo S. Lopes-de-Oliveira,^{*[a]} **György Szalóki**^{*[b]}^[a] Brazilian Biosciences National Laboratory, Campinas, Brazil. E-mail (paulo.oliveira@lnbio.cnpem.br)^[b] Université de Toulouse, Toulouse, France (gyorgy.szaloki@utoulouse.fr)

Confinement of guest molecules within artificial hosts – such as supramolecular cages - offers many potential applications including catalysis, stabilization of reactive species, sensing and delivery. Over the past three decades, many design strategies and tools have been developed that enabled the controlled synthesis of a vast array of cages with tailored properties. Among the *in silico* tools, cavity characterization has not been systematically used, despite being computationally inexpensive and highly informative regarding cavity size and shape. [pyKVFinder](#) was originally developed by our collaborators from the Brazilian Biosciences National Laboratory to identify cavities found in natural hosts such as enzymes. In this context, we have recently adapted [pyKVFinder](#) to supramolecular cages, evaluated its performance (along with other software available for this purpose) and made it available for the supramolecular community.¹

Figure 1. Cavity detected by [pyKVFinder](#) (left), pywindow (middle) and MoloVol (right).

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¹J. S. V. Guerra, L. F. G. Alves, D. Bourissou, P. S. Lopes-de-Oliveira, G. Szalóki *J. Chem. Inf. Model.* **2023**, 63, 3772.

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Development of functionalized self-assembling cyclodextrins for anti-viral purposes

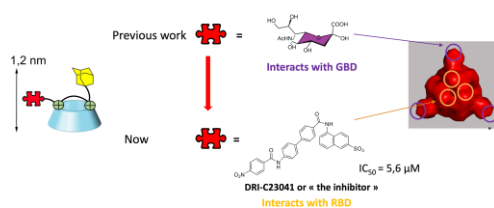
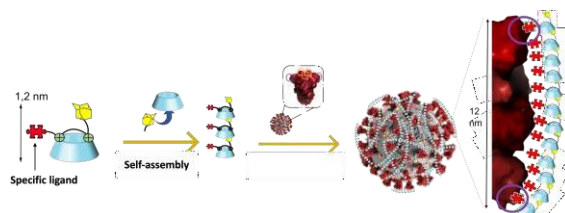
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In order to treat and prevent SARS-CoV-2 infection, several strategies have been developed in recent years, such as vaccination and antiviral drugs. Within the group, we have proposed an alternative strategy by developing cyclodextrin (CD)-based anti-adhesive agents. These modified CDs have an adamantyl function on the primary ring that allows them to self-assemble through a hydrophobic effect and form fibers.¹ In this context, the general approach is to exploit the ability of functionalized CDs to self-assemble and form fibers by covering the virus after attaching to an anchor point, which in this case is the Spike protein. The spike protein is a trimeric protein responsible for the recognition and internalization of the virus by cells. It is composed of two binding domains, the receptor binding domain (RBD) and the glycan binding domain (GBD).² Previously, we synthesized a library of functionalized CDs targeting the GBD by placing sialic acid derivatives on the side chain, and biological studies were conducted, yielding very encouraging results that show antiviral activity. In this work, we proposed changing the anchoring function by replacing it with an inhibitor that will target the RBD.³



Cryptophane-based Cages Towards Xe/Rn Selective Separation

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Dark matter and neutrinos remain among the most important open questions in modern physics. Their study relies on ultra-sensitive **xenon (Xe)** detectors, a noble gas with excellent detection properties. However, the performance of these detectors is strongly limited by the presence of radioactive **radon (Rn)**, which produces undesirable background signals.¹ Due to their very similar physicochemical properties, separating these two noble gases remains extremely **challenging**.

To address this challenge, we build on **cryptophane-type molecular cages**, a class of supramolecular systems known for their strong affinity toward **Xe** and employed in many applications such as ¹²⁹Xe-MRI sensors.² Here, we aim to elegantly tailor new **cryptophane derivatives** with structural modifications designed to **enhance discrimination** between **Xe** and **Rn**. By tuning the cavity size, shape, and chemical environment of these hosts, we seek to better understand and control noble gas **recognition** at the molecular level.

The newly developed **cryptophanes** are then immobilized onto porous solid supports, such as mesoporous silica or MOFs, to generate **hybrid composite materials**. These materials will be characterized and evaluated for their ability to capture **radon** while maintaining **xenon** purity at trace concentrations selectively.

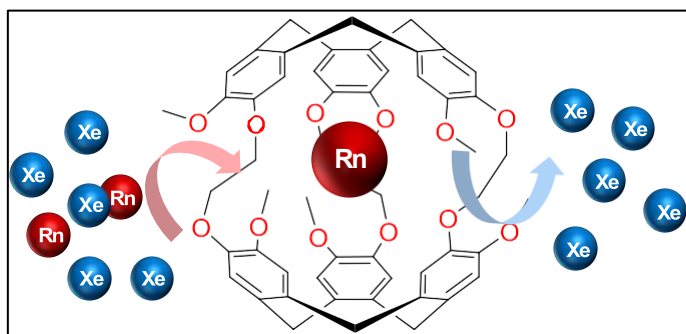


Figure 1: Schematic representation of **Xe/Rn** separation via **cryptophane-based cage**.

Acknowledgements. This work was supported by the National Research Agency (ANR-23-CE31-0022).

¹ H. A. Fogarty, P. Berthault, T. Brotin, G. Huber, H. Desvaux, J.-P. Dutasta, *J. Am. Chem. Soc.* **2007**, *129*, 10332–10333.

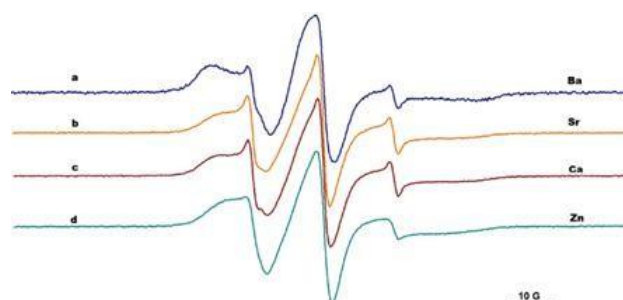
² T. Brotin, J.-P. Dutasta, *Chem. Rev.* **2009**, *109*, 88–130.

Modulation of alginate gels properties through host-guest interactions

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Electron paramagnetic resonance (EPR) spectroscopy represents a sensitive tool that can provide meaningful structural and dynamic insight in various molecular systems with applications in various fields of chemistry, materials science, and the biomedical sciences. The ionotropic alginate-based hydrogels have been explored by various physico-chemical methods in relations with their applications. In this study, the formation of alginate gel from low molecular weight alginate functionalized with β -cyclodextrin (Alg-1,3- β -CD) and adamantane units (Alg-Ad-AT) in the presence of divalent cations (Ca^{2+} , Sr^{2+} , Ba^{2+} , Zn^{2+}) was investigated using EPR spectroscopy (Figure 1). In addition, paramagnetic spin labels (TEMPO units) were covalently attached to the polysaccharide chain. The transition from sol to gel in the presence of divalent cations was monitored by the changes in the dynamics of spin-labelled alginate. The immobilisation of the spin label in the alginate gel reflects the strength of interaction between the cation and alginate chain. The local information provided by EPR parameters of the spin label were correlated with the global information obtained by IR spectroscopy and rheological measurements. Altogether these investigations demonstrated that, although host–guest interactions are not the driving force for the generation of alginate gels, their presence influences and can modulate the gel properties.



The EPR spectra of gels formed by complexation of functionalized alginate in the presence of cations

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Dual Molecular Whirligigs: Synthesis and Actuation

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By introducing a light-driven rotary motor looped in a figure-of-eight molecule (**1B**), our group has provided an initial answer about the quantification of the torque generated by the system (~ 10 pN.nm)^{1,2}. Knowing that such mechanical work could be sufficient to initiate chemical transformations,^{2,3} we designed a more advanced version of this whirligig incorporating two azobenzene photoswitches (**1C**). Azobenzene provides the opportunity to change the ring tension, and thus potentially competing with the motor itself (**1D**). In such a competition, one can in principle quantify the respective forces of the rotary motor and of the switching azobenzenes. Here, we show how to synthesize this new class of dual molecular whirligig for two types of azobenzenes with potentially orthogonal excitation wavelengths⁴. Then, in the second part of this study, we demonstrate effects of the irradiation conditions on the photostationary states and on the relaxation kinetics in the dark. The final objective of this work will be to quantify the respective forces delivered by the motor and the switches, thus bringing valuable insights for the molecular machine community.

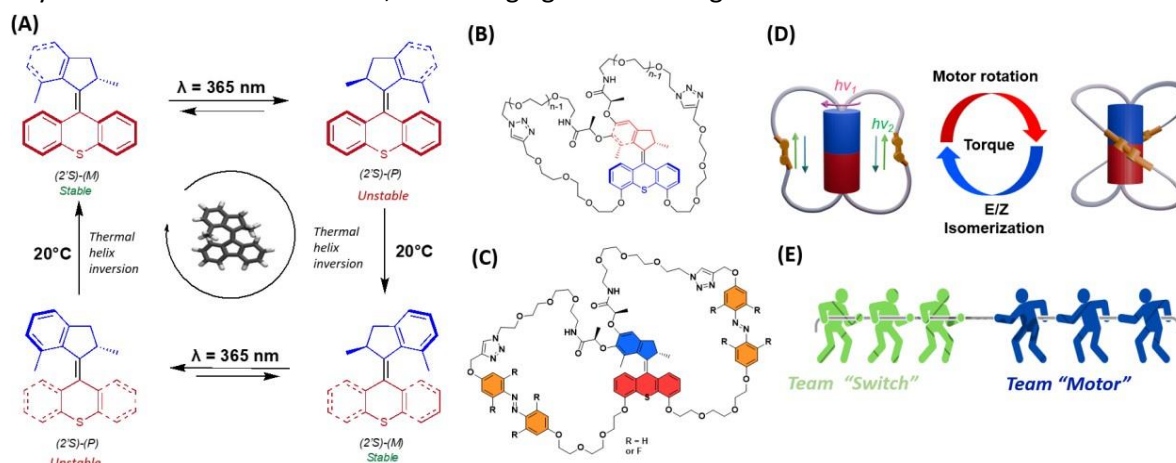


Figure 1. (A) Mechanism of rotation of a molecular motor involving thermal and photochemical steps. Rotor (in blue) and stator (in red); (B) First light-driven molecular whirligig; (C) First dual molecular whirligig incorporating azobenzene; (D) Schematic representation of twisting (under UV irradiation) and untwisting (by thermal relaxation in the dark) of the molecular whirligig; (E) Schematic competition ("tug of war") between the switch and motor.

Acknowledgements. The authors acknowledge the CNRS, the University of Strasbourg, and the Fondation Jean-Marie Lehn for financial support.

¹ N. Koumura, R. W. J. Zijlstra, R. A. van Delden, N. Harada, B. L. Feringa, *Nature* **1999**, *401*, 152-155.

² C. Gao, A. V. Jentsch, E. Moulin, N. Giuseppone, *J. Am. Chem. Soc.* **2022**, *144*, 9845-9852.

³ P. Schiel, M. Maaloum, E. Moulin, I. Nyrkova, A. Semenov, D. Dattler, L.A. Accou, A. Christoulaki, E. Buhler, R. Plamont, J.M. Lehn, N. Giuseppone, *Nat. Nanotechnol.* **2025**, *20*, 1052-1061.

⁴ D. Bléger, J. Schwarz, A. M. Brouwer, S. Hecht, *J. Am. Soc.* **2012**, *134*, 51, 20597-20600.

Peptide-Based Caged Catalysts as Minimalistic Models of Carbonic Anhydrase enzyme

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Metalloenzymes are natural catalysts achieving highly efficient and selective transformations by combining metal active sites with peptide-based binding cavities allowing non-covalent interactions with substrates and reaction intermediates. Although bioinorganic research has demonstrated the critical role of these peptide-based second coordination sphere, these characteristics have not been yet incorporated into artificial catalysts.¹ The majority of synthetic catalysts only mimic the first coordination sphere of given enzymes. Therefore, it is a crucial task to rationally design catalysts confined in a well-defined peptide-based cavity acting as second coordination sphere, especially when it comes to significant societal transformations like CO₂ conversion.²

In this context, we develop bioinspired metal complexes entrapped in organic cages based on the cyclotrimeratrylene (CTV) cap (**Fig.1B**).³ Despite their recent use as bioinspired receptors or catalysts, these artificial cages did not reproduce the amino-acid-based environment found in enzymes. In this project, we therefore aim to design and investigate minimalistic model catalysts featuring Zn metal centers confined within amino acid-decorated cavities, where the Zn (II) center is coordinated by three histidine residues, inspired by the active site of carbonic anhydrase (**Fig.1A**).

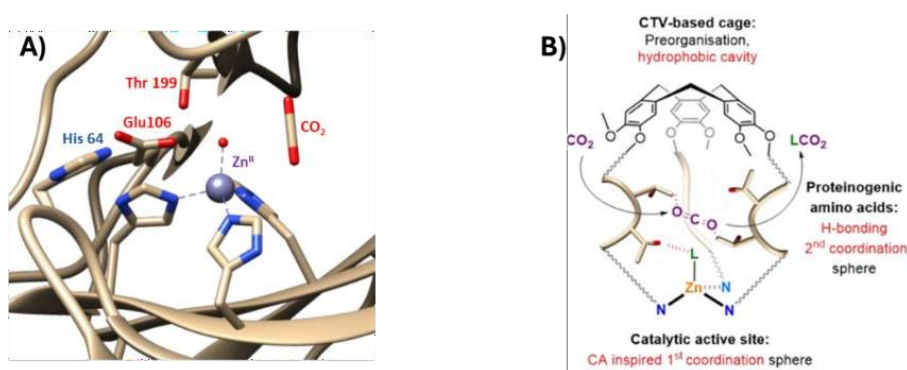


Figure 1: Representation of (A) CA active site with bound CO₂ and (B) the peptide-based caged catalysts target of this study.

This presentation will outline the synthesis and structural design of our amino-acid-functionalized cages, with preliminary catalytic studies using *p*-nitrophenyl acetate (*p*NPA) as a model substrate for hydrolysis reaction.

¹ Zhao, M.; Wang, H.-B.; Ji, L.-N.; Mao, Z.-W. *Chem. Soc. Rev.* **2013**, *42*, 8360–8375.

² Stein, A.; Chen, D.; Igareta, N. V.; Cotelte, Y.; Rebelein, J. G.; Ward, T. R. *ACS Cent. Sci.* **2021**, *7*, 1874–1884.

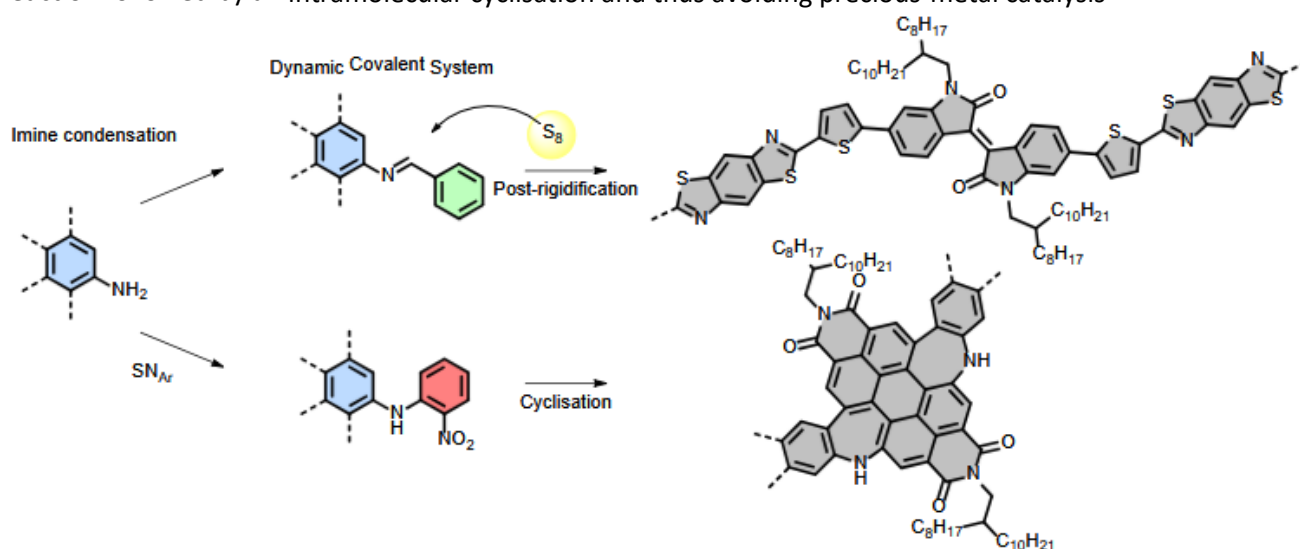
³ Diaio, D.; Simaan, A. J.; Martinez, A.; Colombar, C. *Chem. Commun.* **2023**, *59*, 4288–4299.

New *N*-type Conjugated Polymers for Organic Electronics by Post-Locking Dynamic Covalent Bonds and Metal-Free Synthesis of *N*-incorporating Polyimide Nanographene

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The development of synthetic methods for the obtention of π -conjugated acceptor is a particularly investigated field since these materials were less diversified than their donating counterparts. If it is now state-of-the-art knowledge that these compounds are mainly conjugated polymers synthesised by palladium-catalysed cross-coupling reactions and small molecules such as ITIC and Y6 derivatives,^{1,2} metal-free alternatives are drawing more attention for their lesser economic and environmental impact. While approaches based on dynamic covalent chemistry (DCvC) are paving the road towards stretchable or fully-recyclable materials³ it is at the cost of their stability, which limits their use in organic electronics applications. Our first goal is to post-rigidify imine-based dynamic covalent systems with sulfur, inspired by concepts derived from COF chemistry, allowing us to overcome the stability caveats of classical dynamic materials. It is reported that dynamic imines can irreversibly react with sulfur to afford benzothiazole conjugated motifs. In a second project, we aim to the obtention of GNR-like polymers using amino-PDI as starting material, going first through a S_NAr reaction followed by an intramolecular cyclisation and thus avoiding precious-metal catalysis



Chosen synthetic approaches for the metal-free synthesis of new π -conjugated *N*-type materials.

Acknowledgements. This project was funded by the European Research Council. Analysis were carried out thanks to the SFR Matrix Platform.

- (1) Müllen, K.; Scherf, U. *Macromol. Chem. Phys.* **2023**, 224 (3), 2200337.
- (2) Shao, G.; Liu, H.; Chen, L.; Wu, M.; Wang, D.; Wu, D.; Xia, J. *Chem. Sci.* **2024**, 15 (9), 3323–3329.
- (3) Tran, H.; Feig, V. R.; Liu, K.; Wu, H.-C.; Chen, R.; Xu, J.; Deisseroth, K.; Bao, Z. *ACS Cent. Sci.* **2019**, 5 (11), 1884–1891.

New cycloveratrylene and porphyrin-based cages with application in enantioselective photocatalysis

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Hemicryptophanes are molecular cages well known for their great properties of encapsulation via non-covalent interactions, making them compounds of interest for molecular recognition, catalysis and transport of chemical species.¹ They are based on a functionalized cyclotrimeratrylene (CTV), which is inherently chiral and mostly linked to a variable C_3 -symmetrical moiety. An underused CTV analog is the cyclotetrameratrylene (CTTV),² a chiral assembly of four veratrole units that could give access to C_4 -symmetrical cages. Among the C_4 -symmetrical building blocks, porphyrins are highly valued for their complexation abilities, photophysical properties and have proven their efficiency in catalysis.³

Here, we aim to obtain new molecular cages that combine CTV/CTTV and porphyrin assets in order to perform enantioselective photocatalysis (Figure 1). For this purpose, cages based on porphyrin and CTV have been synthesized, yielding C_1 -symmetrical cages. In parallel, the CTTV based analogs were also studied, paving the way to a new family of C_4 -symmetrical hosts. The obtained cages will be then used for host-guest studies and enantioselective photocatalysis attempts.

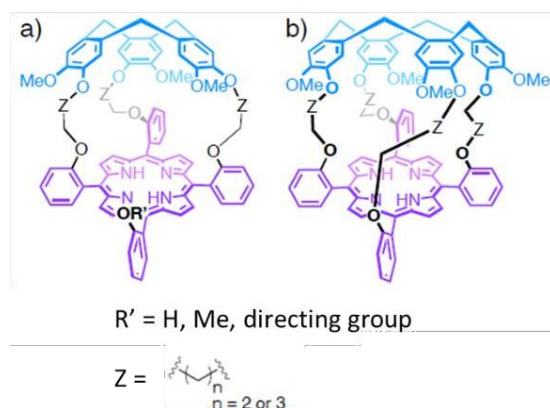


Figure 1: Targeted molecular cages based on a porphyrin and a) a CTV unit or b) a CTTV unit for an application in enantioselective photocatalysis.

Acknowledgements. The authors acknowledge the ANR (ANR-23-CE07-0035 AtropoPhotoCat) for financial support.

¹ Zhang, D.; Martinez, A.; Dutasta, J.-P., *Chem. Rev.* **2017**, *117* (6), 4900–4942.

² White, J. D.; Gesner, B. D., *Tetrahedron Lett.* **1968**, *9* (13), 1591–1594.

³ Rybicka-Jasińska, K.; König, B.; Gryko, D., *Eur. J. Org. Chem.*, **2017**, *2017* (15), 2104–2107.

Synthesis and Study of Bridged Cyclodextrin Regioisomers for Chiral Recognition and Organocatalysis

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This project aims to develop inherently chiral artificial catalysts inspired by nature's ability to achieve high enantioselectivity through the accurate shaping of cavities of protein structures made of only L-aminoacids.^{1,2,3,4} We want to draw inspiration from Nature by designing *D*-sugar-based cyclodextrins (CDs) with asymmetrical bridging⁵ using tris(2-aminoethyl)amine (tren), leading to compounds with mirror-image cavities (Figure 1). Two regioisomers with inherent chiral patterns on the primary rim (ABE and ABD) will be synthesized through a regioselective deprotection of the benzyl ethers on the primary rim. These two structures are expected to direct the formation of opposite enantiomers from the same substrate, mimicking the selectivity of enzymes. The resulting tren-functionalized CDs will be further complexed with metal ions (e.g., Cu(II), Zn(II), Fe(III)) or non-metal ions (e.g., phosphorus) and tested in enantioselective catalysis (e.g., Henry reaction⁶) and chiral molecular recognition (e.g., amino acids). This approach circumvents the tedious synthesis of *L*-sugar-based CDs,⁷ opening new avenues for designing asymmetric catalysts with enzyme-like selectivity.

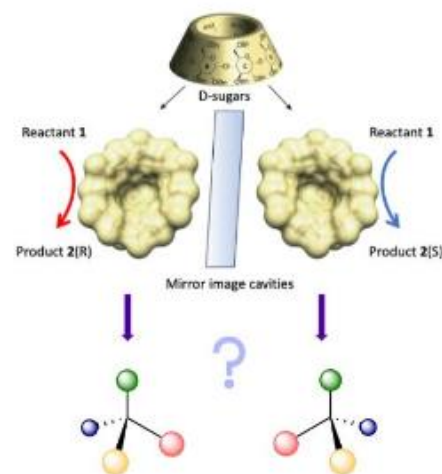


Figure 1. Reshaping of cavities of CDs to achieve enantioselectivity.

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¹ R. Breslow, *Acc. Chem. Res.* **1995**, *28*, 146-153.

² M. S. Robescu, L. Cendon, A. Bacchin, K. Wagner, T. Reiter, I. Janicki, K. Merusic, M. Illek, M. Aleotti, E. Bergantino, M. Hall, *ACS Catalysis*, **2022**, *12*, 7396-7405.

³ F. Botha, J. Budka, V. Eigner, O. Hudeček, L. Vrzal, I. Císařová, P. Lhoták, *Tetrahedron*, **2014**, *70*, 477-483.

⁴ A. Bouchet, T. Brotin, M. Linares, H. Ågren, D. Cavagnat, T. Buffeteau, *J. Org. Chem.* **2011**, *76*, 4178-4181.

⁵ S. Guieu, M. Sollogoub, *J. Org. Chem.*, **2008**, *73* (7), 2819-2828.

⁶ (a) L. Henry, *Comptes rendus*, **1895**, *120*, 1265-1268. (b) Li, J. J. *Springer International Publishing*, Cham, **2021**.

⁷ Y. Wu, S. Aslani, H. Han, C. Tang, G. Wu, X. Li, H. Wu, C. L. Stern, Q.-H. Guo, Y. Qiu, A. X.-Y. Chen, Y. Jiao, R. Zhang, A. H. G. David, D. W. Armstrong, J. Fraser Stoddart, *Nat. Synth.* **2024**, *3*, 698-706.

Kinetically Controlled Unidirectional Molecular Motion in a 2-Station Cyclodextrin Rotaxane

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The development of artificial molecular motors capable of controlled unidirectional motion remains a major challenge due to the stochastic nature of Brownian motion¹. Information ratchet mechanisms have emerged as an effective strategy to bias molecular motion, and cyclodextrin (CD)-based interlocked systems have shown promise in this context. In particular, we have previously demonstrated that directionality can arise from dual kinetic biases in an amine-functionalized CD 3-stations rotaxane. The unidirectionality comes from (i) preferential protection near the wider rim of the conical CD, and (ii) accelerated deprotection mediated by catalytic functionalities on the narrower rim, enabling the CD to effectively “open its own path” along the axle^{2,3}. However, this system suffer from structural complexity and multiple isomeric states, which hinder quantitative kinetic analysis and limit mechanistic understanding.

To overcome this limitation, we have designed a model 2-station rotaxane system with reduced isomeric complexity. This rotaxane was obtained by a regioselective post-functionalization, induced by the functionalized CD, of a symmetrical rotaxane. This design provides a simplified platform for mechanistic studies and enables tuning of the motion rate through controlled CD functionalization, representing a step toward more efficient and programmable synthetic molecular motors.

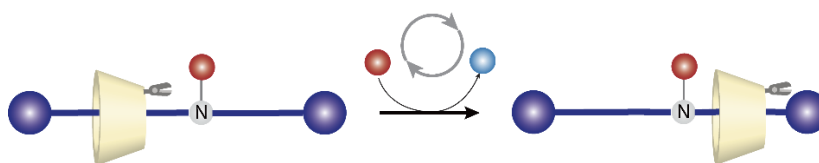


Figure 1. Unidirectional motion of α -cyclodextrin in a two-station rotaxane via an information ratchet mechanism.

Acknowledgements. The authors gratefully acknowledge support from the China Scholarship Council (CSC), Sorbonne Université.

¹ Erbas-Cakmak, S.; Leigh, D. A.; McTernan, C. T.; Nussbaumer, A. L. *Chem. Rev.* **2015**, *115*, 10081–10206.

² Liu, E.; Cherraben, S.; Boulo, L.; Troufflard, C.; Hasenknopf, B.; Vives, G.; Sollogoub, M. *Chem* **2023**, *9*, 1147–1163.

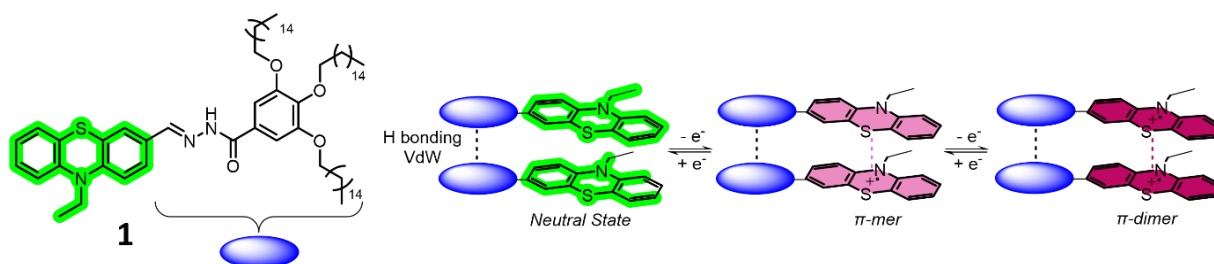
³ Liu, E.; Daou, D.; Hasenknopf, B.; Vives, G.; Sollogoub, M. *Chem* **2025**, *11*, 102623.

A Phenothiazine-based supramolecular gelator for new organic electrode designs

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Organic redox active compounds have received increasing attention for the development of new battery electrode materials due to their high energy density, cycling stability, low toxicity and their potential sustainable production from renewable or petrochemical sources.¹ Despite these advantages, the development of organic electrodes remains constrained by the materials properties that can be accessed by contemporary synthetic design of new (macro)-molecular objects.² Often overlooked, supramolecular design elements however present a great potential to enhance electrode material processability, sustainability and performances.^{2,3} Within this emerging field, we have explored phenothiazine-based low molecular gelators (LMWG) as new electrode active materials. We will present here the use of gelator **1** (see figure) for the design of new organic electrodes. This compound, first reported by Suganaya and coworkers,⁴ can self-assemble in polar solvents classically used for wet electrode processing, allowing to form composite materials structured through a dense supramolecular network. The obtained materials were characterized by electronic microscopy, cyclic voltammetry, UV-Vis, spectroelectrochemistry and constant current cycling, constituting the first electrochemical study of a phenothiazine LMWG-based material. Taking advantage of gelator **1** self-assembly allowed to form electrodes featuring high cycling stability and rate capability in Li half-cell. In a second part we will demonstrate that gelator **1** can also function as redox-active binder, offering an alternative to PVDF for the design of PFAS-free organic electrodes.



Molecular structure of phenothiazine-based gelator(left) and corresponding proposed charge/discharge mechanism (right)

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¹ J. Bitenc, K. Pirnat, O. Lužanin and R. Dominko, *Chem. Mater.*, **2024**, *36*, 1025–1040.

² A. N. Davis, K. Parui, M. M. Butala and A. M. Evans, *Nanoscale*, **2024**, *16*, 10142

³ B. Esser, I. H. Morhenn and M. Keis, *Acc. Mater. Res.*, **2025**, *6*, 6, 754–764

⁴ S. Suganaya, K. Debsharma, E. Ravindran, M. K. Mahato and E. Prasad, *ACS Appl. Polym. Mater.* **2020**, *2*, 3, 1222–1233

Bola-amphiphilic glycodendrimers for targeting glial cells in the brain

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Drug delivery to glial cells in the brain constitutes a formidable challenge, as the blood–brain barrier (BBB) severely restricts the entry of therapeutic agents into the brain, particularly to specific glial cells such as astrocytes and microglia.¹ Intranasal administration as a promising strategy to bypass the BBB and, when combined with nanotechnology, enables direct and targeted delivery to glial cells in the brain.² Dendrimer-based nanosystems are particularly attractive in this context thanks to their uniquely well-defined structure and multivalency confined within nanoscale dimension.³ We therefore designed and synthesized bola-amphiphilic dendrimers bearing glucose (**1a**) and mannose (**1b**) terminals (Figure 1), aiming to selectively target astrocytes and microglia, respectively.^{4,5} These glycodendrimers were synthesized efficiently via a modular double-click (CuAAC) strategy using unprotected carbohydrate units, and self-assembled into supramolecular nanoparticles in water spontaneously. In vivo studies demonstrated that these dendrimer nanosystems indeed achieved selective targeting of astrocytes and microglia, respectively.^{4,5} Our study highlights the potential of bola-amphiphilic glycodendrimers as an effective platform for cell-specific targeting of glial populations in the brain.

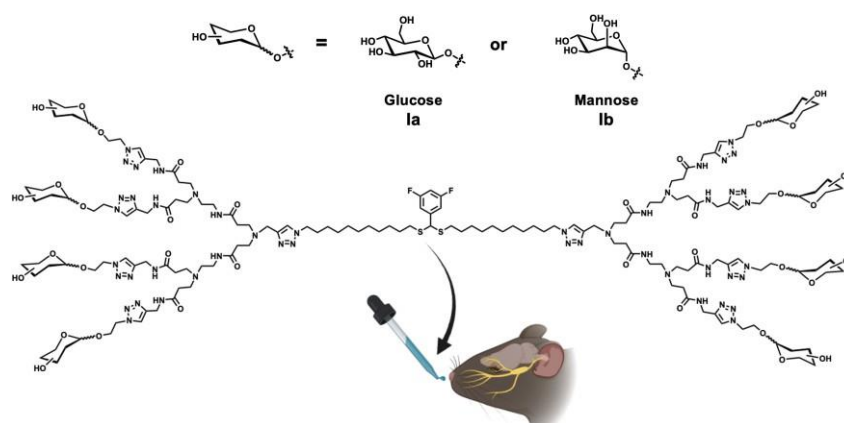


Figure 1. Structures of bola-amphiphilic glycodendrimers and schematic illustration of their intranasal administration for brain delivery.

Acknowledgements. This work was supported by the Horizon Europe Cancer Mission “HIT-GLIO” project (No. 101136835).

1. J. Gao; Z. Xia; S. Gunasekar; et al. *Nat. Rev. Mater.* **2024**, 9(8): 567-588.
2. Y. Chen; C. Zhang; Y. Huang; et al. *Adv. Drug Deliv. Rev.* **2024**, 207, 115196.
3. Q. Ni; J. Wu; C. Galanakou; et al. *Nat. Rev. Bioeng.* **2025**, 3(10): 806-807.
4. Z. Bian; W. Zhang; S. Garofalo; et al. *Nanoscale*, **2025**, 17(48): 27869-27880.
5. Z. Bian; S. Garofalo; L. Shi Qian; et al. **2026**, submitted.

Switchable porphyrin cages: allosteric encapsulation of guests and application to (2)rotaxanes

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Molecular cages are hollow structures with a well-defined three-dimensional cavity that can encapsulate guest molecules or perform reactions in their cavity.(1) Metalloporphyrins are attractive constituents of cages thanks to their various properties and catalytic activities.(2)

Flexible covalent cages, endowed with two zinc(II) porphyrins and eight peripheral 1,2,3- triazolyl ligands were prepared.(3) Coordination of four silver(I) ions to the peripheral ligands switched the cage from a flattened to an open and locked conformation, allowing the allosteric control of encapsulation of neutral guest molecules, such as pyrazine (Figure).(4)

The receptor properties of our covalent cages can be leveraged for the assembly of (2)semiro- taxanes4b and (2)rotaxanes, since such control of the threading step or macrocycle translation by effector binding to additional sites has rarely been reported.(5)

Acknowledgements.

Financial support from the ANR (project "Switchables cages" ANR 14-CE06-0010), The Ministry of Education and Research, LabEx-CSC and the GDR MAPYRO are gratefully acknowledged.

(1) M. Yoshizawa, J. K. Klosterman, M. Fujita, *Angew. Chem. Int. Ed.* **2009**, *48*, 3418.

(2) S. Durot, J. Taesch, V. Heitz, *Chem. Rev.* **2014**, *114*, 8542.

(3) a) L. Kocher, S. Durot, V. Heitz, *Chem. Commun.* **2015**, *51*, 13181; b) L. Schoepff, L. Kocher, S. Durot, V. Heitz, *J. Org. Chem.* **2017**, *82*, 5845.

(4) a) R. Djemili, L. Kocher, S. Durot, A. Peuronen, K. Rissanen, V. Heitz, *Chem. – Eur. J.* **2019**, *25*, 1481. b) R. Djemili, S. Adrouche, S. Durot, V. Heitz, *J. Org. Chem.* **2023**, *88*, 14760.

(5) a) J. Kuwabara, C. L. Stern, C. A. Mirkin, *J. Am. Chem. Soc.* **2007**, *129*, 10074;

b) S. Cantekin, A. J. Markvoort, J. A. A. W. Elemans, A. E. Rowan, R. J. M. Nolte, *J. Am. Chem. Soc.* **2015**, *137*, 3915; c) D. S. Marlin, D. González Cabrera, D. A. Leigh, A. M. Z. Slawin, *Angew. Chem. Int. Ed.* **2006**, *45*, 1385; d) F. Durola, V. Heitz, F. Reviriego, C. Roche, J.-P. Sauvage, A. Sour, Y. Trolez, *Acc. Chem. Res.* **2014**, *47*, 633.

Synthesis and optoelectronic investigations of promising intermolecular anionic mixed-valence BACD and azaBPDI based compounds

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We recently demonstrated that *ortho*-pentannulated bisazacoronene diimides (or BACDs) are strongly self-assembling in solution. Cyclic voltammetry investigations revealed that these compounds spontaneously form two unexpected anionic mixed-valence (MV) and π -dimer states in dissociative chlorinated solvents, where the large splitting of the first reduction wave is related to highly stabilized MV states.¹ There are not much examples of fully organic compounds that show spontaneous self-assembly into purely intermolecular anionic mixed valence states in the literature, making this type of compounds interesting to investigate for their potential to behave as efficient organic semi-conductors.

o-pentannulated BACDs are synthesized following a sequence of white light-driven photocyclization as an alternative to the Pictet-Spengler reaction, followed by oxidative rearomatization, and a Pd-catalysed *ortho*-pentannulation.² They are easily tuneable, allowing us to change electronic, geometric and regioisomeric parameters in order to stabilise the MV state as much as possible. azaBenzannulated perylene diimides (or azaBPDI)s, which are easier to synthesize and purify than BACDs, are presented here as models, and their optoelectronic properties were compared to highlight the most promising structural features to synthesize the best corresponding BACDs candidates. Then, the MV state properties of these molecules will be investigated in materials such as polymers, functionalized surfaces and more.

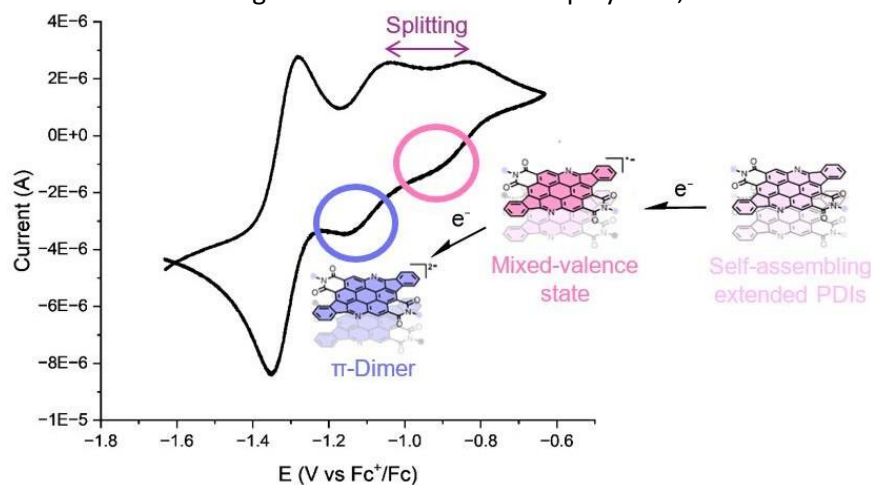


Figure 1. Cyclic Voltammetry (0.1 M Bu_4NPF_6 , 100 mV/s) in DCM with Fc (0.1 mM) as an internal reference, showing a large splitting of the first reduction wave, leading to a highly stable MV state.

¹ A. H. G. David, M. Roger, O. Alévêque, H. Melnychenko, L. Le Bras, M. Allain, A. Gapin, D. Canevet, O. Ségut, E. Levillain, A. Goujon, *Angew. Chem. Int. Ed.* **2025**, *64* (1), e202413616.

² A. Goujon, L. Rocard, T. Cauchy, P. Hudhomme, *J. Org. Chem* **2020**, *85* (11), 7218–7224.

Supramolecular Transformation Between Saddle And Crown Conformations Of A New Cyclotribenzylidene CTB-1NH-pyridine, Driven By Acylation Or Metal Coordination

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Cyclotribenzylidene derivatives (CTBs) are bowl-shaped chiral macrocyclic trimers presenting a C_3 - symmetry.¹ Known since decades, these compounds have been used as sensors,² and as building blocks for the design of liquid crystals.³ They are known to acquire two energy-minimum conformations, a rigid crown and a flexible saddle (**Figure 1a**).⁴ Recently, our group described the preparation of C_1 -symmetrical CTB containing a nitrogen atom(s) in place of one of the methylene bridges (**CTB-1NH**, **CTB-2NH**, **Figure 1b**).⁵ In recent years, we have focused on the supramolecular transformation of these compounds between saddle and crown conformations, particularly through alkylation or acylation of the nitrogen bridge. We also investigated their physicochemical properties, especially their conformation in solution and in the solid state, as well as their solubility. We will present the latest results on the newly synthesized CTB, the **CTB-1NH-py** (**Figure 1c**), of particular interest as, to our knowledge, represents the first CTB incorporating a pyridine unit in its backbone in addition to a nitrogen bridge. Taking advantage of these two functional groups, we are investigating a supramolecular transformation between saddle and crown conformations, either by acylating the nitrogen bridge (**Figure 1d**) or by coordinating the pyridine to metal centers (**Figure 1e**).

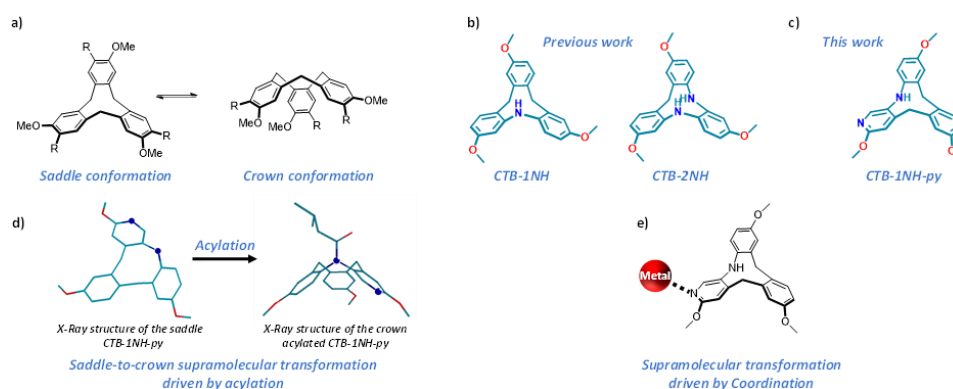


Figure 1. a) Saddle and crown conformations adopted by CTBs, b) previously reported CTBs developed by our team incorporating a nitrogen bridge(s), c) a new CTB “CTB-1NH-py” featuring both a nitrogen bridge and a pyridine unit, d) supramolecular transformation from the saddle to the crown conformation driven by acylation, with the corresponding X- ray crystal structures (hydrogens omitted for clarity), e) coordination of CTB-1NH-py to a spherical representation of the metal center.

¹ A. Collet, *Tetrahedron*, 1987, **43**, 5725–5759.

² P. F. Fernandes and D. R. Mishra, *Asian J. Chem.*, 2020, **32**, 2139–2142.

³ S. Chen, H. Guo, X. Geng and F. Yang, *J. Mol. Liq.*, 2018, **252**, 145–150.

⁴ H. Zimmermann, P. Tolstoy, H. H. Limbach, R. Poupko and Z. Luz, *J. Phys. Chem. B*, 2004, **108**, 18772–18778.

⁵ C. Vigier, D. Fayolle, H. El Siblani, J. Sopkova- de Oliveira Santos, F. Fabis, T. Cailly, E. Dubost, *Angew. Chem. Int. Ed.*, 2022, **134**, e202208580.

Towards Electron-Responsive Supramolecular Hydrogels

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Thomas Gibaud,^[b] Floris Chevallier,^[a] Denis Frath,^[a] Christophe Bucher^[a]

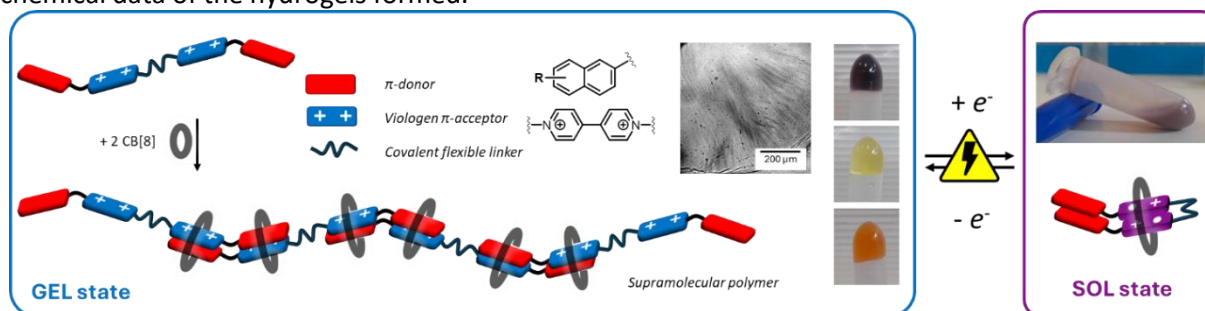
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Interest in stimuli-responsive soft materials has grown over the last decade. Hydrogels, in particular, have been the subject of extensive research because of their many potential applications.^[1] Gels can be defined as solvent trapped in a network that typically contribute little to the mass. One key feature of supramolecular gels, involving a network of non-covalent bonds, is their ability to undergo self-healing processes or to respond to external stimuli. (pH, T, P, light). These soft, dynamic and responsive supramolecular materials have already proved useful in many fields, from catalysis to electronics.^[2]

Our project aims at addressing two challenges in the field of responsive hydrogels linked to the following observations: 1) Most stimuli-responsive behaviors reported so far come from serendipitous finding due to a lack of control and anticipation over the molecular events involved in the gelation process; 2) Responsiveness to electrical stimuli remains almost unexplored, despite being essential to ensure implementation of such materials in devices.

Over the last few years, our group has developed major expertise in the characterization and engineering of electro-switchable gels.^[3-6] This poster will focus on supramolecular gels formed by the spontaneous self-assembly of cucurbit[8]urils host with π -conjugated donors and electron-responsive bipyridinium acceptors.^[7] The mechanisms of formation and response to stimulation will be discussed on the basis of spectroscopic, rheological, microscopic and electrochemical data of the hydrogels formed.



[1] L. Voorhaar, R. Hoogenboom, Chem. Soc. Rev., 2016, 45, 4013–4031.

[2] H. Wu, et al., J. Adv. Mater., 2019, 31(12), 1806204.

[3] C. Kahlfuss et al., Chem. Eur. J., 2018, 24, 13009–13019.

[4] S. Chowdhury et al., J. Phys. Chem. B, 2021, 125(43), 12063–12071.

[5] C Roisard et al., ECS Adv., 2022, 1, 020502.

[6] V. Andrieux et al., J. Mater. Chem. C, 2023, 11, 12764–12775.

[7] Y. Liu et al., Angew. Chem. Int. Ed., 2010, 49, 6576–6579.

Using supramolecular chemistry to perform (2+2) photocycloadditions in solid-state organic synthesis

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Cyclobutane synthesis often involves a (2+2) photoaddition where regiochemistry can be difficult to control in intermolecular solution-based reaction. Principles of crystal engineering enable reactant alkenes to be organized in the solid state to undergo intermolecular (2+2) photodimerizations that generate desired products selectively and in near quantitative yield. Small molecules that act as supramolecular templates can be used to form cocrystals and position reactant alkenes within the 4.2 °Å distance for a (2+2) photocycloaddition to occur.(1) Understanding the crystal packing of a molecule is, therefore, important to understand its solid-state reactivity. Challenging cyclobutanes in the form of polycyclobutanes (e.g., ladderanes) and cyclobutane rings fused with even larger ring systems (i.e., 5- and higher) are emerging as important building blocks in medicinal and materials chemistry, as well as the chemistry of natural products. Moreover, there is a need to develop approaches that provide ready and efficient access to such products.(2) In this work, we report the study of the synthesis of fused tricyclic hydrocarbon core of adjacent 4- and 6-membered rings through (2+2) photodimerizations performed in the organic solid state.(3) We approach the design of the starting alkenes by understanding the crystal packing and chemical reactivity.

(1) Macgillivray, L. R. *J. Org. Chem.* 2008, 73 (9), 3311–3317

(2) a) Meibom, A.; Sleep, N. H.; Chamberlain, C. P.; Coleman, R. G.; Frei, R.; Hren, M. T.; Wooden, J. L. *Nature* 2002, 419, 705–708 b) Epplin, R. C.; Paul, S.; Herter, L.; Salome, C.; Hancock, E. N.; Larrow, J. F.; Baum, E. W.; Dunstan, D. R.; Ginsburg-moraff, C.; Fessard, T. C.; Brown, M. K. *Nat Commun* 2022, 13 (6056), 1–5 c) Kolk, M. R. Van Der; Janssen, M. A. C. H.; Rutjes, F. P. J. T.; Blanco-ania, D. *ChemMedChem* 2022, 17, e202200020

(3) Green, B. S.; Schmidt, G. M. J. *Tetrahedron Lett.* 1970, 11 (49), 4249–4252

Guest Exchange by a Partial Energy Ratchet in Water

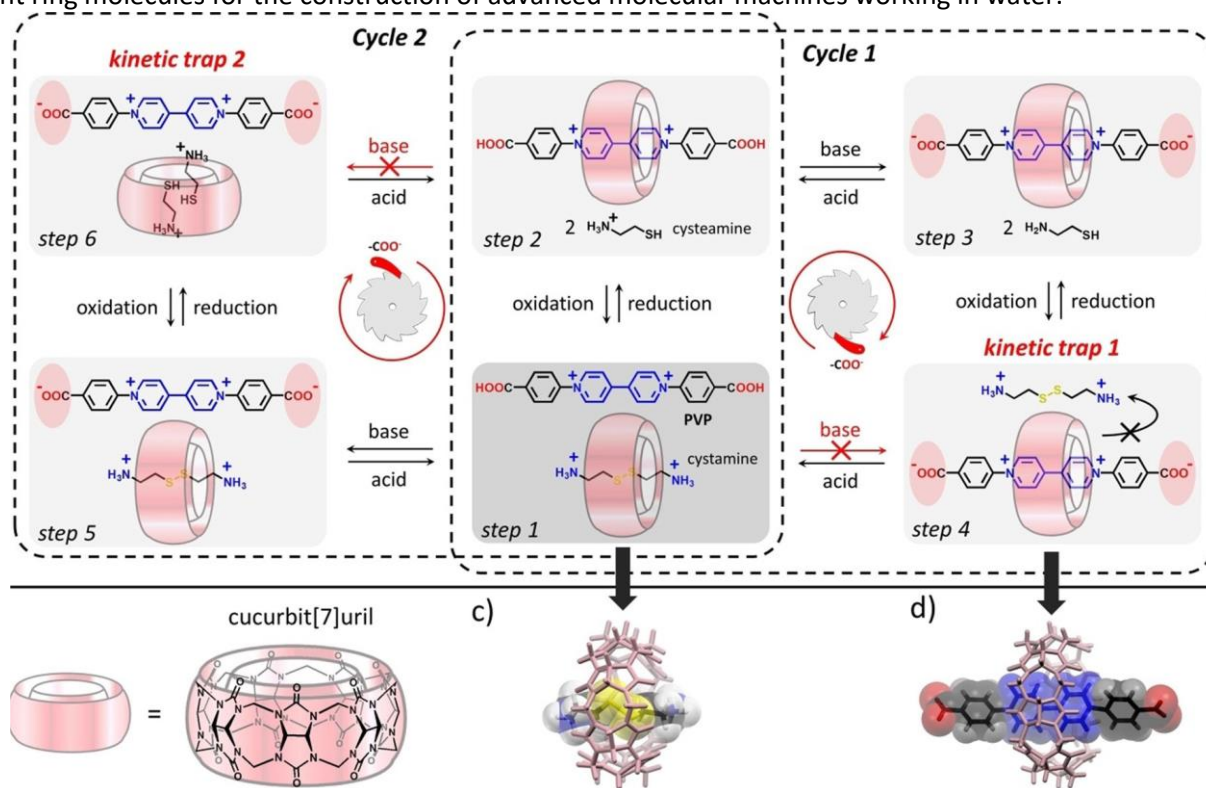
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Molecular machines are ubiquitous in nature and function away from equilibrium by consuming fuels to produce appropriate work. Chemists have recently excelled at mimicking the fantastic job performed by natural molecular machines with synthetic systems soluble in organic solvents.¹⁻³ In efforts toward analogous systems working in water, we show that guest molecules can be exchanged in the synthetic macrocycle cucurbit[7]uril by involving kinetic traps, and in such a way as modulating energy wells and kinetic barriers using pH, light, and redox stimuli.⁴ Ditolyl-viologen can also be exchanged using the best kinetic trap and interfaced with alginate, thus affording pH-responsive blue, fluorescent hydrogels. With tunable rate and binding constants toward relevant guests, cucurbiturils may become excellent ring molecules for the construction of advanced molecular machines working in water.



1. S. Erbas-Cakmak, D. A. Leigh, C. T. McTernan and A. L. Nussbaumer, Artificial Molecular Machines, *Chem. Rev.*, 2015, **115**, 10081-10206.
2. S. Kassem, T. van Leeuwen, A. S. Lubbe, M. R. Wilson, B. L. Feringa and D. A. Leigh, Artificial molecular motors, *Chem. Soc. Rev.*, 2017, **46**, 2592-2621.
3. A. Kermagoret and D. Bardelang, The Diversity of Cucurbituril Molecular Switches and Shuttles, *Chem. Eur. J.*, 2023, **29**, e202302114.
4. X. Yang, Q. Cheng, V. Monnier, L. Charles, H. Karoui, O. Ouari, D. Gignes, R. Wang, A. Kermagoret and D. Bardelang, Guest Exchange by a Partial Energy Ratchet in Water, *Angew. Chem. Int. Ed.*, 2021, **60**, 6617-6623.

Toward Understanding Substituent-Controlled Excited-State Behavior in Hemicyanine Dyes

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Hemicyanine dyes are promising photoresponsive chromophores whose optical and photochemical properties can be tuned through structural modification. In this work, a series of stilbazolium-type hemicyanine derivatives with varying substitution patterns is investigated to understand how substituent type, position, and multiplicity influence excited-state behavior in solution. The study combines experimental NMR spectroscopy, UV-vis absorption and fluorescence spectroscopy^{1,2} with time-dependent density functional theory calculations to relate spectroscopic behavior to underlying electronic and structural features³. The project is focused on identifying structure-property relationships relevant to photoisomerization and competing excited-state pathways in polar media. Particular attention is being given to the role of substitution pattern, medium effects, and the balance between electronic redistribution and geometric response following excitation. In parallel, the work also examines how the supramolecular environment may influence pathway selection and photochemical outcome^{4,5}. This combined experimental and computational approach is intended to provide a broader framework for understanding substituent-controlled photoresponse in hemicyanine systems and to guide the future design of dyes with tunable excited-state properties. Ongoing work includes extending the spectroscopic dataset, conducting medium-dependent studies, and further analyzing excited-state properties to elucidate the factors governing reactivity in this class of compounds.

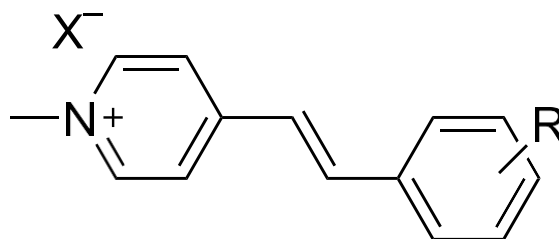


Figure 1: General structure of the quaternary hemicyanine dyes.

¹Görner, H.; Fojtik, A.; Wróblewski, J.; Currell, L. J. VIII. *Z. Für Naturforschung A* **1985**, *40* (5), 525–537.

² Abdel-Halim, S. T. *J. Lumin.* **2011**, *131* (1), 30–35.

³ Huix-Rotllant, M.; Park, W.; Mazaherifar, M.; Choi, C. H. *Theor. Chem. Acc.* **2025**, *144* (6), 41.

⁴ Gromov, S. P.; Vedernikov, A. I.; Kuz'mina, L. G.; Kondratuk, D. V.; Sazonov, S. K.; Strelenko, Y. A.; Alfimov, M. V.; Howard, J. A. K. *Eur. J. Org. Chem.* **2010**, *2010* (13), 2587–2599.

⁵ Kang, Y.; Tang, X.; Yu, H.; Cai, Z.; Huang, Z.; Wang, D.; Xu, J.-F.; Zhang, X. *Chem. Sci.* **2017**, *8* (12), 8357–8361.

Harnessing Multi-Stranded Helices for Molecular Links and Topological Hydrogels

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Natural biomolecules such as DNA can switch between single-, double-, triple- and quadruple- helical conformations to regulate their functions. Synthetic multi-stranded helices^{1,2} provide a powerful platform for designing topologically complex architectures³ with similar dynamic features. Our group has recently reported the synthesis of an oligo(*m*-phenylene ethynylene) strand that self-assembles into a double- and a triple-helix in aqueous environments. The equilibrium between these helices is concentration- and temperature-dependent.

In this work, we use these helices as a scaffold to construct entangled soft materials⁴ Terminal reactive groups were introduced to cross-link multiple helices with PEG-based linkers and form 3D entangled hydrogels through click reactions. We expect this approach will help us understand how entanglements influence hydrogel morphology and mechanical properties. In parallel, we are also exploring whether the upper and lower rims of the helices can be connected to form discrete molecular links.

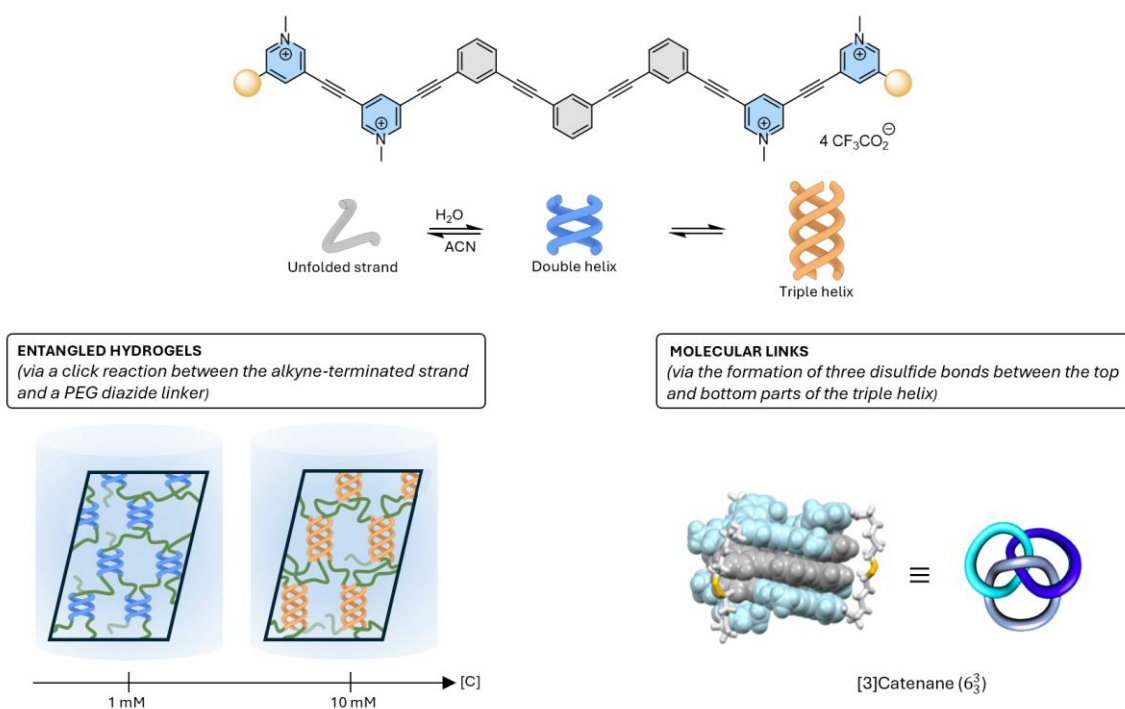


Figure 1: Schematic overview from helical self-assembly to entangled materials and molecular links.

¹ D. J. Hill, M. J. Mio, R. B. Prince, T. S. Hughes, J. S. Moore, *Chem. Rev.* **2001**, *101*, 3893-4012.

² J. Shang, Q. Gan, S. J. Dawson, F. Rosu, H. Jiang, Y. Ferrand, I. Huc, *Org. Lett.* **2014**, *16*, 4992-4995.

³ Z. Ashbridge, E. Kreidt, L. Pirvu, F. Schaufelberger, J. H. Stenlid, F. Abild-Pedersen, D. A. Leigh, *Science* **2022**, *375*, 1035-1041.

⁴ (a) J. Kim, G. Zhang, M. Shi, Z. Suo, *Science* **2021**, *374*, 212-216. (b) C. Liu, N. Morimoto, L. Jiang, S. Kawahara, T. Noritomi, H. Yokoyama, K. Mayumi, K. Ito, *Science* **2021**, *372*, 1078-1081.

Sergeants & Soldiers approach for chirality control in gels of supramolecular nanotubes of Ln³⁺ based 1D coordination polymers

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Coordination polymers are highly tunable and versatile objects opening real perspectives in the technological use of these unique systems. In particular, peculiar magnetic and chiroptical properties can be observed on lanthanide–radical chains with original topologies such as helical chains.^{1,2} Unfortunately, their surface deposition is tricky and restrain their uses. A strategy is to form metallogels of supramolecular nanotubes out of these objects using radicals with long alkyl chains such as 2-(4'-(octadecyloxy)phenyl)-4,4,5,5-tetra-methylimidazolin-1-oxyl-3-oxide (NIT-C18).^{3,4} Herein, we demonstrate that the chirality of the supramolecular nanotubes can be controlled using (R/S)-2-(4'-(octadecan-2-yloxy)-4,4,5,5-tetramethylimidazolin-1-oxyl-3-oxide (NIT-C₁₈(R/S)) radicals. We also show that the combination of chiral and achiral radicals in a Sergeant & Soldiers approach allows the formation of enantiomerically pure nanotubes which can be deposited on surface via wet chemistry techniques. Thus, it gives a hint to better control their supramolecular organisation on surface.

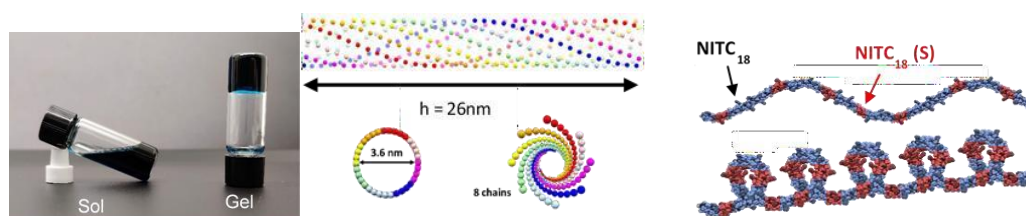


Figure 1 Left: Gelation test. Middle: Supramolecular nanotube representation extracted from SAXS measurements. Right: Sergeant & Soldiers 1D coordination polymer.

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¹ K. Bernot, *Eur. J. Inorg. Chem.* **2023**, e202300336.

² F. Houard, Q. Evrard, et al. *Angew. Chem.-Int. Ed.* **2020**, 59, 780-784.

³ F. Houard, A. Olivier, et al. *J. Mater. Chem. C* **2024**, 12, 3228-3237.

⁴ F. Houard, G. Cucinotta, et al. *Mater. Horiz.* **2023**, 10, 547-555.

Understanding the Scope of Perfluorophenyl-Phenyl Interactions: Crystal Engineering of the [2+2] Photodimerization

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The ability to reliably assemble alkenes in the solid state to undergo covalent-bond-forming **[2+2] photodimerization** can allow chemists to form molecules that are inaccessible in solution. The formation of covalent bonds in crystals is relevant to both organic synthesis (e.g., green chemistry) and materials science (e.g., information storage). The **perfluorophenyl-phenyl interactions** have been widely studied in many contexts such as crystal and co-crystal assembly using various linkers between these aryl groups (such as amides, alkenes and alkynes) as well as 4 and 4' functionalization to further help direct the orientation of the molecules.¹

This presentation focuses on as-of-yet unreported systems: the use of partially fluorinated asymmetric stilbenes (presenting 3 to 7 fluorine atoms). These systems are shown to reliably crystallize following various patterns and regularly respect Schmidt's criteria. These species thus steadily undergo [2+2] photodimerization in the solid state with **quantitative yields of a single product** (fig. 1). Several interactions dictate the way fluorinated stilbenes stack to form crystals and undergo reaction. These include H-F and F-F dipolar interactions as well as π -stacking. These interactions can be tuned by varying the number and position of fluorine atoms on the stilbenes to lead to the desired stacking and photodimerization product, with both pure compounds and co-crystals.

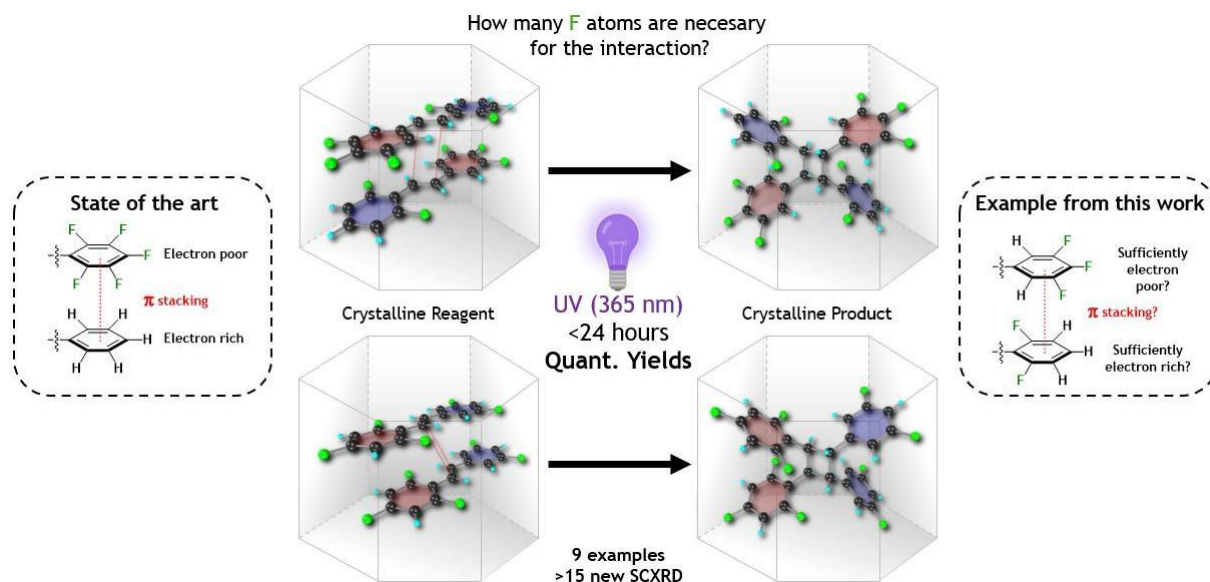


Figure 1. Solid-state [2+2] photodimerization of polyfluorinated stilbenes to the corresponding cyclobutane

Gotta Catch 'Em All: New Amphoteric Nitrogen-Containing Cryptophanes for Selective Trapping of Toxic Thallium(I)

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The contamination of ecosystems by thallium(I) ions, mainly resulting from coal combustion and mineral extraction, represents a significant environmental concern due to the extreme toxicity of Tl(I) even at trace levels (less than 1 µg/L in fresh water and 1–88 µg/L for a water near metal mining).¹ Developing efficient methods for its detection and removal from water is therefore essential.^{2,3}

Among potential molecular receptors, cryptophanes stand out for their tunable cavities and versatile functionalization⁴. Phenolate-substituted cryptophanes have shown strong affinity toward Tl(I) but only under basic conditions and with poor selectivity over alkali metals such as K⁺ ions.⁵ Introducing other heteroatoms, particularly nitrogen or sulfur, offers a promising route to improve Tl(I) encapsulation at neutral pH.^{6,7}

Based on recent promising results, demonstrating the beneficial role of aromatic amines in Tl(I) binding, we have developed new synthetic strategies with gram-scale access to nitrogen-containing cryptophanes with complete *anti*-diastereoselectivity, without the need for column chromatography. The influence of various nitrogen-protecting groups has been investigated to optimize the synthesis. This robust platform paves the way for designing new amphoteric cryptophanes capable of selectively capturing Tl(I) ions in aqueous media at neutral pH.

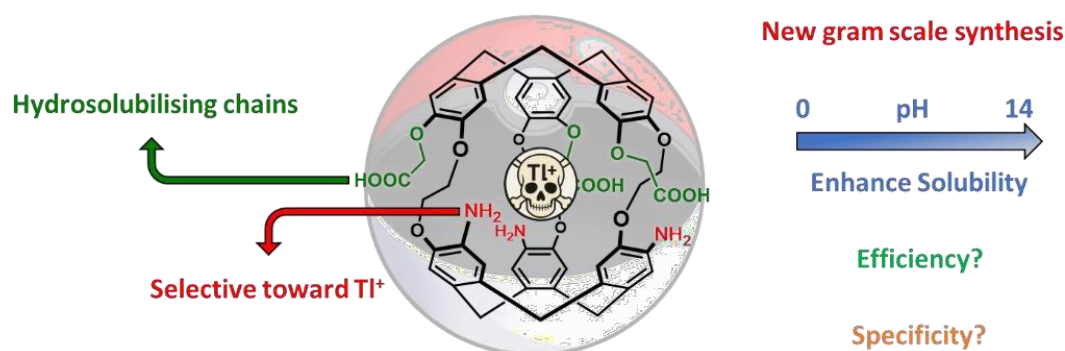


Figure 1 : New amphoteric cryptophane for Tl⁺ ions trapping in water.

References

1. J. Fujihara, N. Nishimoto, *Current Research in Toxicology*. **2024**, *6*, 100157.
2. D. Giaiotti. *Atmospheric Pollut. Res.* **2018**, *9*, 502.
3. V. Zitko, *Sci. Total Environ.* **1975**, *4*, 185.
4. S. Kancherla, J.H. Hansen, *Eur. J. Org. Chem.* **2024**, *27*, e202301050.
5. T. Brotin, *et al*, *J. Phys. Chem. B* **2012**, *116*, 10905.
6. M. Doll, *et al*, *J. Org. Chem.* **2022**, *87*, 2912.
7. R. Benchouaia, *et al*, *J. Org. Chem.* **2024**, *89*, 4560.

Kinetic studies of light-driven whirligigs

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Light-driven molecular motors are molecules able to convert photons into unidirectional motion, in a four step process, by first a *E-Z* photoisomerization, followed by a thermal helix inversion. Repeating those two-step leads to a 360° rotation¹. When those molecules are integrated into a polymer network, UV light can trigger the actuation of the soft material indicating that the continuous rotation of the motor entangles the polymer chains, bringing the motor units closer to each other². In a previous work,³ our group developed an 8-shaped molecular motor, where two polymer chains are looped between the rotor and stator parts. Under light irradiation, rotation leads to the formation of more constrained isomers, as indicated by UPLC-MS kinetic measurements, resulting in the storage of elastic energy in the system. In the absence of light, the rotation in the opposite direction is promoted as elastic energy is released. In this work, we propose to study the influence of the chain length in the ring to evaluate whether the system could store more elastic energy, as it should be dependent on the number of entanglements. To do that, we developed new light-driven molecular whirligigs with different sizes of looped chains, and we probed the relaxation process for each new whirligig using UPLC-MS and UV-Vis kinetic measurements. We also study the influence of the light power and of the temperature on the photostationary state.

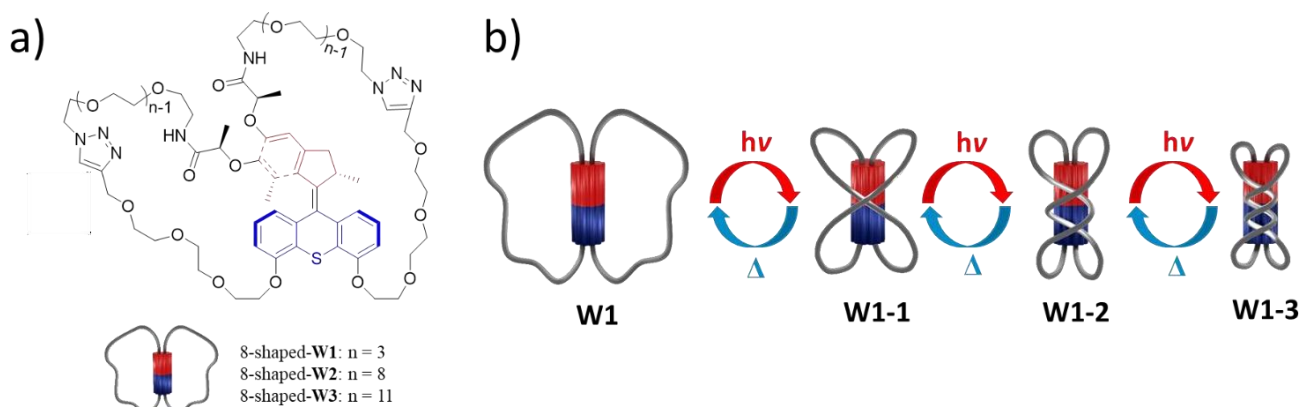


Fig. 1 (a) Molecular structure and (b) Functioning principle of the molecular whirligig.

Acknowledgements. This work was developed within the project *Photomorph* (Grant No ANR-24-CE06-7386.) granted by the French National Research Agency (ANR).

(1) Koumura, N.; Geertsema, E. M.; van Gelder, M. B.; Meetsma, A.; Feringa, B. L. *J. Am. Chem. Soc.* **2002**, *124* (18), 5037–5051. <https://doi.org/10.1021/ja012499i>.

(2) Li, Q.; Fuks, G.; Moulin, E.; Maaloum, M.; Rawiso, M.; Kulic, I.; Foy, J. T.; Giuseppone, N. *Nature Nanotech* **2015**, *10* (2), 161–165. <https://doi.org/10.1038/nnano.2014.315>.

(3) Gao, C.; Vargas Jentzsch, A.; Moulin, E.; Giuseppone, N. *J. Am. Chem. Soc.* **2022**, *144* (22), 9845–9852.

Target-Directed Dynamic Combinatorial Library of Cyclic Peptides for Biomolecular Recognition

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Peptides are attractive compounds for targeting complex biological systems. Their intermediate size between small molecules and biologics offers favourable pharmacokinetics and membrane permeability, while maintaining high specificity and binding affinity. Cyclic peptide scaffolds (e.g. β -Hairpin, α -Helix), in particular, show enhanced stability and pharmacological performance compared to linear analogues, making them especially promising therapeutic candidates. Yet, their design using traditional structure-guided rational approaches is limited by the availability of crystal or solution structures and often require labor-intensive optimization processes. To overcome these challenges, we have been developed two strategies based on **Dynamic Combinatorial Chemistry (DCC)**, to create peptide libraries weather optimizing the staple geometry,¹ or the side-chain functions of cyclic peptides.² In both strategies, peptide scaffolds are functionalized with thiol groups present in cysteine residues, allowing **dynamic exchange processes with thioester building blocks** to generate dynamic combinatorial libraries (DCL).

Here, we present a proof of concept where these libraries can be selectively enriched in the presence of a biological target (e.g. proteins, glycosaminoglycans), enabling a **target-directed DCC (td-DCC)** approach for efficient biomolecular recognition and drug discovery.

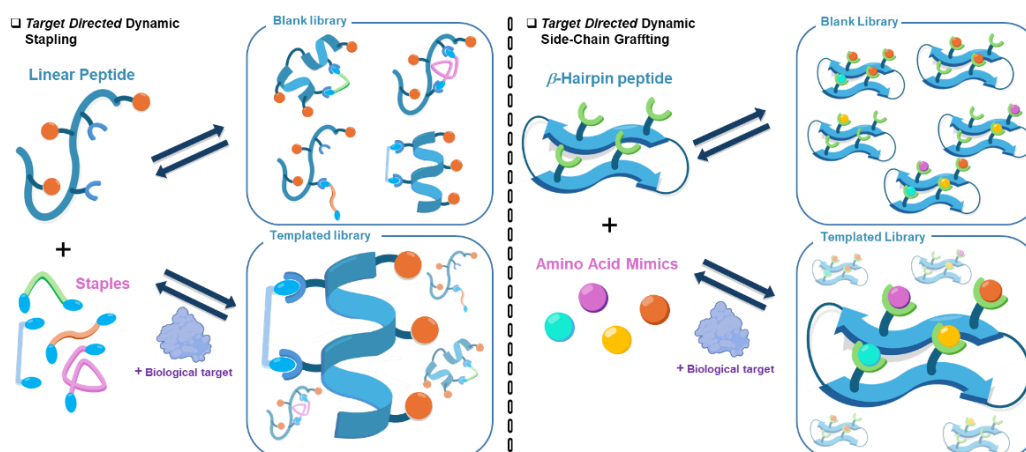


Figure 1. td-DCC approaches based on cyclic peptides allowing biomolecular recognition.

¹ A. Rodrigues, J. Garcia Coll, D. Ravault, B. Zagiel, L. Carlier, L. Rocard, R. Mounné, *ChemRxiv* **2026**, 15000968/v1

² B. Zagiel, T. Peker, R. Marquant, G. Cazals, G. Webb, E. Miclet, C. Bich, E. Sachon, R. Mounné, *Chem. Eur. J.* **2022**, 28, e202200454

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