

Mach-5 2024

MOLECULAR **M**ACHINERY:
MAKING • **M**EASURING • **M**ODELLING



“Rocca Vescovile”
Bertinoro • Italy
1 – 4 September 2024

The Conference

Hosted in the beautiful fortress of Bertinoro (Rocca Vescovile), on a hill that dominates the Pianura Padana and the Adriatic coast of the Emilia-Romagna region, the conference is the second event of a biannual conference series on the fascinating topic of molecular machinery, after the meeting hold at the Plön castle, Germany, in September 2022.

Topics

Mach-5 welcomes young scientists active in the field of artificial molecular machines and their components (motors, switches, rotors, actuators ...). Studies of these systems within the 3M (modelling, making and measuring) are welcome, as well as contributions focused on the functions that can arise from coupling of molecular machines to an energy source or trigger (light, redox, concentration gradient, electric, magnetic fields, etc.) and their interaction with the environment (solution, surface, polymers, biological systems, etc.).

Scope

Mach-5 aims at creating a scientific forum on the various theoretical and experimental aspects related to the design, development and application of molecular machinery. The event is focused on the involvement and support of young investigators, defined as scientists at the beginning of their independent research career, after the PhD, but before a tenured position.

Opening Remarks

Miniaturization of electronic and magnetic devices spurred unprecedented technological developments in information processing and storage. As a consequence, the progress in microelectronics exerts an increasing impact on modern societies. Downscaling mechanical devices and machines is expected to have a similar technological and societal impact. Although the field is still under development, research in the past three decades has shown that the concepts of macroscopic devices and machines can be transferred to the molecular or supramolecular level. Moreover, it has become evident that applications of molecular devices and molecular machines, enabled by appropriately integrating/interfacing them with their surroundings, could provide radically innovative solutions to significant problems in many areas of technology and medicine. The scientific maturity of this research and its great potential for breakthrough applications were testified by the award of the Nobel Prize in Chemistry 2016 to three founding fathers of the field, namely, Jean-Pierre Sauvage, Fraser Stoddart and Ben Feringa.

To foster the exchange of ideas, particularly among young scientists, the emergence of ground-breaking visions and the recognition of creativity in a burgeoning research field, the Mach-5 conferences series was launched in Europe in 2022, along with scientific prizes – the Sauvage-Stoddart-Feringa Awards - named after the three Nobel laureates in Chemistry for molecular machines.

The first event of the series was held in the Plön castle, Germany, on 11-14 September 2022, co-chaired by the two of us. The meeting was opened with a conference from Ben Feringa, and plenary lectures were delivered by Vincenzo Balzani (SSF Senior Awardee) and Víctor García-López (SSF Junior Awardee). About 40 young researchers animated the scientific program with outstanding presentations and intense discussions throughout the week.

We are now pleased and proud to present, again as co-chairs, the second conference of the series, hosted in Bertinoro, Italy. The beautiful venue consists of a medieval castle and a guest house (formerly a Bishop fortress) and is managed by the University Residential Centre of Bertinoro, whose stakeholders are the University of Bologna and the municipality of Bertinoro. The 2024 edition will be opened by Nobel laureates in Chemistry Prof. J.-M. Lehn (1987) and Prof. J.-P. Sauvage (2016), lecturing not only on their scientific results but also on the importance of mentorship and integrity in scientific research. The program comprises two plenary contributions from the 2024 SSF Senior and Junior Awardees – Nathalie Katsonis and Yunyan Qiu, respectively – as well as 27 lectures and 8 short presentations, and is complemented by a rich social program. Young scientists are the main protagonists at Mach-5 conferences, and none of the speakers should have a permanent position. Our aim is to provide visibility to young researchers at the stage of their career when they need it most.

While we are working on setting up Mach-5 as a firmly established series of conferences, an informal tradition seems to have emerged: the Mach-5 events must be held in a castle. Although this requirement sets a high standard for the future, there is no doubt that the Old Continent can offer a wide choice of such venues in all its countries.

Enjoy the meeting!



Alberto Credi
Mach-5 Co-chairs



Rainer Herges

Program

	Sunday 1 September	Monday 2 September	Tuesday 3 September	Wednesday 4 September
Morning (9:00-12:30)	Travel	Breakfast	Breakfast	Breakfast
		E. Del Grosso	C. Bezuidenhout	B. Schmidt
		F. Rizzuto	J. Sheng	S. Maiti
		D. Pooler	W. Danowski	S. Fielden
		J. Seale	N. Durandin	Y. Feng
		Coffee break	Coffee break	Coffee break
		E. Penocchio	A. Özcelik	I. Neira Garcia
		S. Borsley	Y. Gisbert	A. Blanco Gómez
		F. Nicoli	R. Toyoda	L. von Krbek
		A. Businski / L. Andreoni	C. Taticchi / M. Gerdson	G. Capocasa
Lunch time	Lunch	Lunch	Lunch Closing remarks	
Afternoon (14:00-19:00)	Arrival and registration Opening remarks	Senior SSF Award N. Katsonis	Excursion / Free time	Departure
	Inspirational lecture J.-M. Lehn (open to public)	Junior SSF Award Y. Qiu		Travel
	Inspirational lecture J.-P. Sauvage (open to public)	Coffee break		
	Roundtable discussion	A. Saady		
		B. Roberts		
		S. Amano		
	Get-together party	R. Plamont		
		Short break		
		L. Casimiro		
		E. Liu / P. Gallagher		
Dinner	C. Lee / M. Ovalle	Conference dinner		

Lectures (20 minutes)

Communications (10 minutes)

Conference Schedule

1 September 2024

14:00 • Arrival and Registration

14:30 • Opening remarks

Institutional greetings from the University of Bologna by Alberto Credi

Welcome by Rainer Herges

Inspirational Lectures | *Chairperson: Alberto Credi*

14:40 • **Prof. Jean-Marie Lehn**
Molecular Motions - A Panorama

15:40 • **Prof. Jean-Pierre Sauvage**
From water splitting research to catenanes, knots and molecular machines

16:40 • Roundtable discussion | *Moderators: Alberto Credi, Rainer Herges*

17:30 • Welcome Cocktail

2 September 2024

Session 1 | *Chairperson: Cristian Pezzato*

9:00 • **Erica Del Grosso**
Dissipative DNA-based systems

9:20 • **Felix Rizzuto**
Photo-control of DNA assemblies through time and space

9:40 • **Daisy Pooler**
Making and Breaking Photo-Responsive Artificial Molecular Machines

10:00 • **James Seale**
Active transport of macrocycles into micelles using artificial molecular pumps

10:20 • Coffee Break

Session 2 | *Chairperson: Giulio Ragazzon*

11:10 • **Emanuele Penocchio**
Power strokes in molecular motors: Predictive, irrelevant, or somewhere in between?

11:30 • **Stefan Borsley**
Putting catalysis to work

11:50 • **Larissa von Krbek**
Switchable macrocycles and cages

Short presentations (10'):

12:10 • **Artjom Businski**
Promising Diazocine Compounds for Hybrid Smart Materials

12:20 • **Leonardo Andreoni**
Novel prototypes of multistable [2]- and [3]rotaxanes

12:30 • Lunch

Sauvage-Stoddart-Feringa Award Lectures | *Chairperson: Rainer Herges*

Senior SSF Awardee:

14:00 • **Nathalie Katsonis**
Mechanochemistry of molecular machines

Junior SSF Awardee:

15:00 • **Yunyan Qiu**
The Rise and Promise of Artificial Molecular Machines in Polymer Chemistry and Materials Science

16:00 • Coffee Break

Session 3 | *Chairperson: Andreas Vargas Jentzsch*

16:20 • **Abed Saady**
A platform approach to mechanically caged molecules

16:40 • **Benjamin Roberts**
Information ratcheting information

17:00 • **Shuntaro Amano**
Repurposing a catalytic cycle for transient self-assembly

17:20 • **Rémi Plamont**
Out-of-Equilibrium Mechanical Disruption of β -Amyloid-Like Fibers using Light-Driven Molecular Motors

17:40 • Short Break

Session 4 | *Chairperson: Robert Hein*

17:50 • **Lorenzo Casimiro**
A Molecular Primum Mobile

Short presentations (10'):

18:10 • **Enxu Liu**
Molecular information ratchets exploiting the asymmetry of functionalized cyclodextrins for autonomous active transport

18:20 • **Peter Gallagher**
The Hitchhiker's Guide to Mechanical Stereochemistry

18:30 • **Christopher Lee**
Operation of Artificial Molecular Pumps in Water

18:40 • **Marco Ovalle**
Influence of geometrical photoisomerization in dynamic self-assembly

19:00 • Dinner

3 September 2024

Session 5 | *Chairperson: Zbigniew Pianowski*

9:00 • **Charl X. Bezuidenhout**
Ultra-Fast Molecular Rotor Dynamics: from isolated to densely packed rotor layers

9:20 • **Jinyu Sheng**
Pushing light-driven molecular motors towards perfection

9:40 • **Wojciech Danowski**
Shining Light on Porous Solids

10:00 • **Nikita Durandin**
Triplet-Sensitized Isomerization of Azoswitches

10:20 • Coffee Break

Session 6 | *Chairperson: Stefano Crespi*

11:10 • **Ani Özcelik**
A Hemithioindigo Molecular Motor Operating by Constitutional Alteration and Hydrogen Bonding

11:30 • **Yohan Gisbert**
Coupling Rotary Motion to Helicene Inversion within Molecular Motors

11:50 • **Ryojun Toyoda**
Photoluminescence for Molecular Machines and Devices

Short presentations (10'):

12:10 • **Chiara Taticchi**
Wavelength-steered motion in an autonomous light-driven molecular rotor

12:20 • **Mirko Gerdson**
Magnetic Levitation Controlled by Light

12:30 • Lunch

14:00 • Free Time in Cervia

18:30 • Guided tour of the Cervia Salt Pan (Saline di Cervia)

19:00 • Social dinner

Session 7 | *Chairperson: Nadja Simeth*

- 9:00 • **Bernd Schmidt**
Mechanoresponsive Metal-Organic Cages
- 9:20 • **Subhabrata Maiti**
Tuning Biocolloidal Taxis and Catalysis in Gradient of (Oligo)nucleotides
- 9:40 • **Stephen Fielden**
Controlled fusion of polymer nanoparticles
- 10:00 • **Yuanning Feng**
Molecular Motors Driven by Electrons and Protons
- 10:20 • Coffee Break

Session 8 | *Chairperson: Stefano Corrà*

- 11:10 • **Iago Neira**
Light-driven ratcheted self-assembly of diastereomeric host-guest systems
- 11:30 • **Arturo Blanco Gómez**
Modulation of Mechanical and Nanostructural Properties of a pH-Responsive Self-Assembled Hydrogel
- 11:50 • **Federico Nicoli**
Design and characterization of complex reaction networks in dynamic mechanically interlocked molecules
- 12:10 • **Giorgio Capocasa**
Beyond Acid-Base Reactions: Interfacing Activated Carboxylic Acids with Electrical Circuits
- 12:30 • Closing remarks and lunch

Inspirational Lectures

Prof. Jean-Marie Lehn

University of Strasbourg | France

Nobel Laureate 1987



Prof. Jean-Marie Lehn is the father of supramolecular chemistry. His research involves the study of non-covalent interactions between molecules. Lehn's groundbreaking research has significantly advanced our understanding of molecular recognition and self-assembly processes which are at the basis of the vital chemical functions in living organisms. His work has laid the foundation for numerous applications in materials science, medicine, and nanotechnology and his contributions were recognized by the 1987 Nobel Prize in Chemistry along with Donald Cram and Charles Pedersen. He currently is Professor at the University of Strasbourg, and director of the "Laboratoire de Chimie des Interactions Moléculaires" at the Collège de France in Paris.

Prof. Jean-Pierre Sauvage

University of Strasbourg | France

Nobel Laureate 2016



Prof Jean-Pierre Sauvage is a pioneer of chemical topology. Sauvage's research focuses on mechanically interlocked molecules such as catenanes and rotaxanes. He developed the high-yielding synthetic approaches to catenanes and other mechanically interlocked molecules, such as the molecular trefoil knot, which are fundamental in the development of nanotechnology and molecular machines. He was awarded the Nobel Prize in Chemistry, along with J. Fraser Stoddart and Ben Feringa, in 2016 for their contributions to field of molecular machines. He currently is Emeritus Professor at the University of Strasbourg, and emeritus research director of the CNRS in Strasbourg.

Sauvage-Stoddart-Feringa Award Lectures

Prof. Nathalie Katsonis

University of Groningen | The Netherlands

Senior SSF Awardee 2024



The research of Prof. Katsonis focuses on the transmission of motion from the molecular to the macro-scale aiming at 'Active Molecular Systems and Materials'. Her achievements have provided the underpinnings for increasingly complex functionalities in dynamic and ultimately life-like supramolecular materials.

Since 2020 she is Professor of chemistry at the Stratingh Institute of Chemistry of the University of Groningen (the Netherlands).

Prof. Yunyan Qiu

National University of Singapore | Singapore

Junior SSF Awardee 2024



Prof. Qiu aims at applying synthetic organic, polymer, macrocyclic and supramolecular chemistry to the design and synthesis of functional dynamic materials and catalysts for environmental, energy, and nature-inspired biomedical applications.

Since 2022 he is Presidential Young Professor at the National University of Singapore where he leads the Laboratory of Dynamic Materials.

Dissipative DNA-based systems

Erica Del Grosso,^a Leonard J. Prins,^b Francesco Ricci^a

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^b Department of Chemical Sciences, University of Padua, Via Marzolo 1, 35131 Padua, Italy.

A strong current interest in the field of Supramolecular Chemistry is the development of artificial molecular devices that mimic dissipative behavior and exhibit life-like properties. Adaptation, metabolism and evolution are just a few examples of how Nature uses chemical energy to sustain life under dissipative conditions.

In the last years, synthetic DNA has proven to be an extraordinary biomaterial for the development of dissipative artificial systems. In the emerging field of Dissipative DNA Nanotechnology, several strategies have been presented to introduce dissipative control over synthetic DNA-based devices.¹ For example, we have shown that it is possible to use Allosteric as a key strategy to engineer DNA nanomachines for transient loading and releasing of molecular cargos. Recently, we have also demonstrated a novel strategy to introduce dissipative control over the toehold-mediated strand displacement process.² This is one of the most widely used reactions in the field of DNA Nanotechnology that allows to introduce this type of behavior in a variety of different DNA systems that generally operate under thermodynamic conditions.

We have thus demonstrated the possibility of achieving pulse-like behavior in a DNA-based reaction, but also the dissipative decoration of polymeric DNA nanostructures and the chemically-fueled reorganization of these DNA nanostructures.

References

1. E. Del Grosso, E. Franco, L. J. Prins, F. Ricci. *Nat. Chem.* **2022**, *14*, 600-613.
2. E. Del Grosso, P. Irmish, S. Gentile, L. J. Prins, R. Seidel, F. Ricci. *Angew. Chem. Int. Ed.* **2022**, *61*, e202201929.

Photo-control of DNA assemblies through time and space

Willi Ragnar Berg,^a Yasmin Khazid,^a Laura Wimberger,^a Jonathon Beves,^a Felix Rizzuto^a

^a School of Chemistry, University of New South Wales, Sydney, Australia 2052

ABSTRACT

Time is the lens through which all action occurs, but at the nanoscale it gets challenging to control how machines change shape and move over time – programming when, how long, and over what distances they operate requires control over reaction timescales.

In this talk, I'll discuss how visible light, small molecules, and protons can be used synergistically as stimuli to create non-equilibrium DNA architectures and nanomachines. Our technique is broadly applicable to individual DNA and RNA strands, micron-length DNA-based polymers, and transformable DNA origami.¹⁻³ Molecular binders can be leveraged to control the lifetime of DNA origami transformations, modulating their operation in both spatial and temporal domains. We can now form recyclable bio-compatible polymers and actuate DNA origami away from equilibrium, enabling new possibilities in tissue scaffolding, delivery, and sensing technologies.

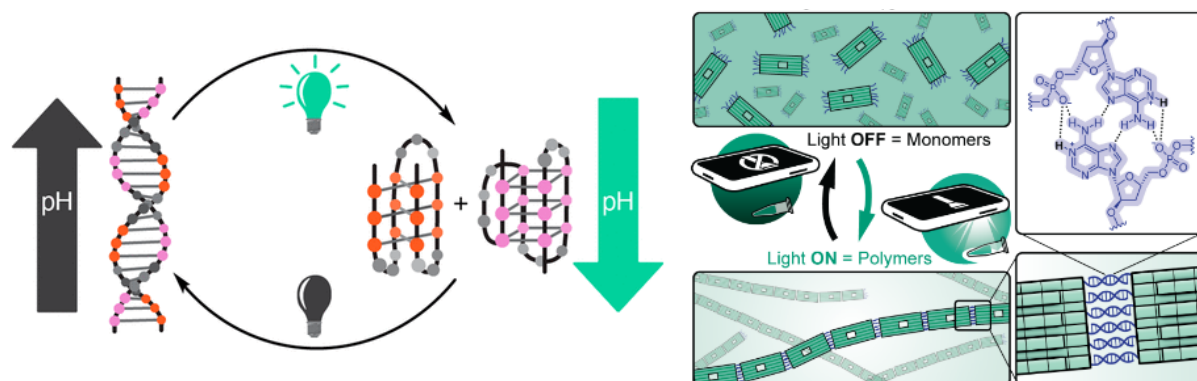


Figure 1. Light can control the morphology of discrete (left) and polymer (right) architectures.

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Making and Breaking Photo-Responsive Artificial Molecular Machines

Daisy R. S. Pooler

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Controlling motion of molecules at the nanoscale has been an aspiration for scientists for many years; the rise of *molecular machines* over the past few decades has shown that it is possible to achieve this goal. The 2016 Nobel Prize in Chemistry was awarded to pioneers in this field, for work on *light-driven rotary molecular motors* and *mechanically interlocked molecules*.

Light-driven rotary molecular motors are able to continuously rotate in a single direction when irradiated with light. Extensive research has elucidated the exact rotation mechanism of these motors, and we better understand how to tune their rotational properties, such as speed and efficiency.¹ However, there are some challenges that must be addressed before light-driven molecular motors can find utility beyond scientific research; they are typically powered by high energy UV light, which is unsuitable for applications in biology. In addition, they are typically inefficient and they difficult to synthesise on a large scale. During my PhD work at the *University of Groningen*, we aimed to address these challenges through the development of *heterocyclic light-driven rotary molecular motors*.^{2,3}

Mechanically interlocked molecules (MIMs) consist of multiple components connected via mechanical bonds, which allow independent movement of the components with respect to each other, but prevent their dissociation. In my current position at *KTH Royal Institute of Technology* (Stockholm), we are working towards constructing photo-responsive MIMs for use in biological settings – using the mechanical bond as protective armour to improve the longevity of biomolecules.

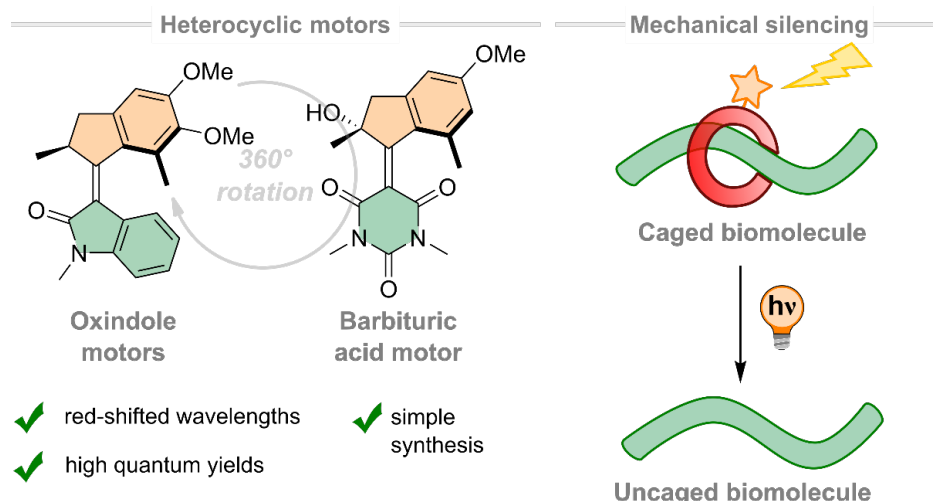


Figure 1. Left: Heterocyclic light-driven rotary motors included in this talk, and their advantages. Right: Using the mechanical bond as a protective armour for mechanical silencing of biomolecules.

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2. D. R. S. Pooler, D. Doellerer, S. Crespi, B. L. Feringa, *Org. Chem. Front.* **2022**, *9*, 2084–2092.
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Active transport of macrocycles into micelles using artificial molecular pumps

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During the past decade, researchers have created a variety of artificial molecular pumps capable of the active transport of macrocycles from free solution to mechanically interlocked states. In their ability to drive nonequilibrium transport, these artificial molecular pumps resemble natural transmembrane transporters, which are widespread in living organisms. But despite this functional and mechanistic resemblance, rotaxane-forming molecular pumps have not yet been demonstrated operating in aqueous self-assemblies in imitation of their biological counterparts. Here, we report that rotaxane-forming molecular pumps can effect the active transport of charged macrocycles from aqueous solution into polymeric micelles. The micelles remain stable after rings have been pumped into them, indicating that rotaxane-forming pumps can operate on self-assembled matter without incurring the disintegration of the assemblies. The pumping of rings, however leads to increases in the average micellar diameter (11.6 to 13.8 nm) as measured by DLS and the average zeta potential (+43.8 to +54.7 mV). By quantitative ¹H NMR spectroscopy, the micellar pumping efficiency is found to be 65%, as compared to 91% in an equivalent small-molecule (nonmicellar) control experiment. This disparity in pumping efficiency is attributed to diminished formation of the key host-guest complex in the first stage of pumping in the micellar experiments. Spin-spin relaxation time (T_2) measurements and ¹H DOSY NMR allow characterization of the micellar microstructure and record that the diffusion rate of macrocycles is reduced fivefold upon being pumped from free solution to micelle-bound states.

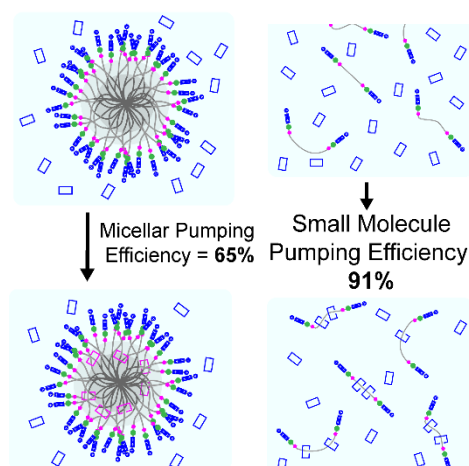


Figure 1. The operation of molecular pumps appended to micelles (left) occurs with reduced efficiency compared to their operation as unimeric small molecules (right).

Power strokes in molecular motors: Predictive, irrelevant, or somewhere in between?

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For several decades, molecular motor directionality has been rationalized in terms of the free energy of molecular conformations visited before and after the motor takes a step, a so-called power-stroke mechanism with analogues in macroscopic engines. Despite theoretical and experimental demonstrations of its flaws, power-stroke language is quite ingrained, and some communities still value power-stroke intuition. By building a catalysis-driven motor into simulated numerical experiments, we here systematically report on how directionality responds when the motor is modified accordingly to power-stroke intuition. We confirm that the power stroke mechanism does not generally predict the directionality. Nevertheless, the simulations illustrate that the relative stability of molecular conformations should be considered as a potential design element for adjusting the motor bias. Though power strokes are formally unimportant for determining directionality, we show that practical attempts to alter a power stroke have side effects that can in fact alter the bias. The change in the bias can align with what power-stroke intuition would have suggested, offering a potential explanation for why the flawed power-stroke concept can retain an apparent utility when engineering specific systems.

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Putting catalysis to work

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Most chemists do catalysis to get their hands on the product of a reaction. As molecular mechanists, we can largely ignore the product, and instead get our hands on a much more juicy prize: the free energy released from the catalysed reaction.¹ The link between catalysis and molecular machines has been well-demonstrated,² with the synthesis of artificial autonomous chemically fuelled motors³ and pumps⁴ becoming increasingly routine. Such machines, which function through a catalysis-driven information ratchet mechanism,⁵ underpin the most sophisticated known nanotechnology (called biology).

Biology uses these machines in virtually every single example of task performance. By contrast, in the early 21st century, artificial catalysis-driven machines instead float around in solution, providing proof-of-concept platforms for mechanistic studies, but are currently largely useless for driving any sort of useful processes.⁵ While making these machines is undeniably a lot of fun, it seems likely that we might one day have to start seriously thinking about how to use such machines for useful task performance as the basis of our own artificial nanotechnology; in other words, we must learn how to put catalysis to work.

In this talk, I will discuss some of the unique tasks that ratchets can achieve (i.e. going beyond switching),⁵ and discuss a recent example catalysis-driven ‘work’ with a molecular motor.⁶ I will then look forward and discuss some of the challenges and opportunities that might arise from translating the principles of molecular ratchets to compartmentalized systems.⁷

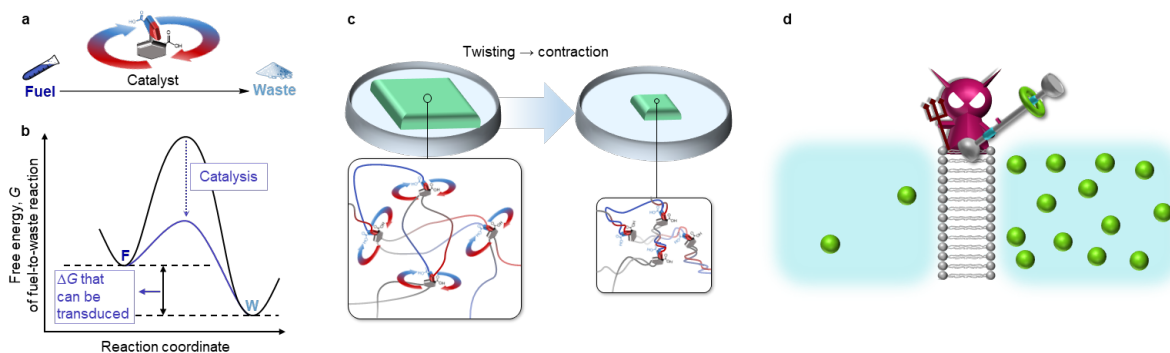


Figure 1. Putting catalysis to work. **a** Motors are catalysts. **b** Catalysis lets us access some of the free energy of the fuel-to-waste reaction. **c** We can harness this energy to perform work, e.g. powered gel contraction. **d** How can we translate these principles to compartmentalized systems.

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Switchable macrocycles and cages

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Photoswitchable molecules can reversibly interconvert between two different isomers. With new applications for photoswitches constantly emerging, the necessity arises to continue to develop photoswitches with different properties than the already established ones. We have developed a versatile synthesis for macrocyclic azobenzenes, which allows for facile modification of these photoswitches. One example (Figure 1, left) shows high chemical stability, long half-life of its *Z*-isomer, quantitative *Z*→*E* conversion under white light, and excellent separation of the excitation bands to address either the *E* or *Z*-state selectively. Almost quantitative *Z*→*E* conversion, even under white light, is a unique feature with an important impact on applications, in which the configuration under ambient light needs to be close to 100%.¹

Inclusion of photoswitchable azobenzene units as spacers into ditopic bridging ligands **L^m** and **L^p**, containing two chelating pyrazolyl-pyridine termini, allows formation of metal complex assemblies with Co(II) that undergo a range of light-induced structural transformations. One notable result is the light induced conversion of a Co₂(**L^p**)₃ dinuclear triple helicate (based on the *E* ligand isomer) to a C₃-symmetric Co₄(**L^p**)₆ assembly, assumed to be an edge-bridged tetrahedral cage, based on the *Z* ligand isomer. Another is the preparation of a series of Co₄(**L^m**)₆ complexes, of which Co₄(*E*-**L^m**)₆ was crystallographically characterised and consists of a pair of Co₂(**L^m**)₂ double helicates connected by an additional two bridging ligands which span the pair of helicate units, giving a cyclic Co₄ array in which one and then two bridging ligands alternate around the periphery. A set of Co₄(**L^m**)₆ complexes could be prepared containing different ratios of *Z* : *E* ligand isomers (0 : 6, 2 : 4, 4 : 2 and 6 : 0) of which Co₄(*Z*-**L^m**)₂(*E*-**L^m**)₄ was particularly stable and dominated the speciation behaviour, either during light-induced switching of the ligand geometry in pre-formed complexes, or when ligand isomers were combined in different proportions during the preparation. These examples of (i) interconversion between Co₂L₃ (helicate) and (ii) Co₄L₆ (cage) assemblies with **L^p**, and the interconversion between a series of Co₄L₆ assemblies Co₄(*Z*-**L^m**)_n(*E*-**L^m**)_{6-n} with **L^m**, constitute significant advances in the field of photoswitchable supramolecular assemblies.²

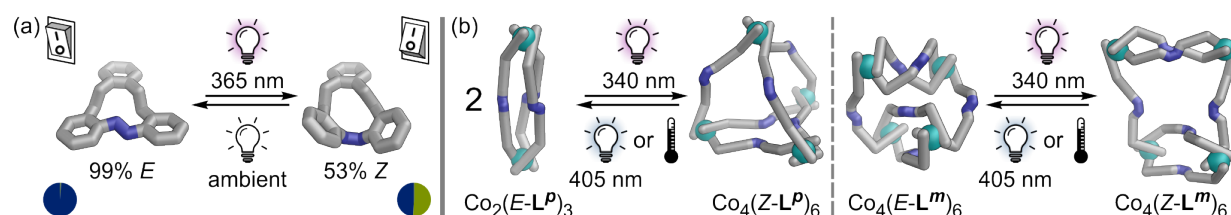


Figure 1. (a) A macrocyclic photoswitch. (b) Two metallo-supramolecular assemblies which can change their structure upon irradiation with UV light.

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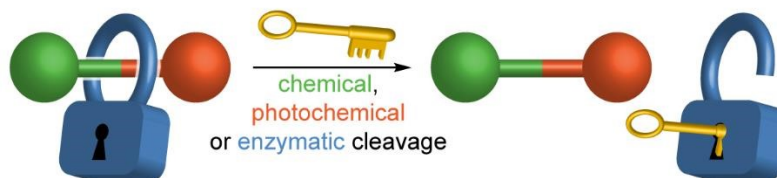
A platform approach to mechanically caged molecules

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Mechanically interlocked molecules (MIMs) such as rotaxanes and catenanes¹ have been transformed from mere synthetic curiosities to functional materials with practical applications in a range of fields: artificial molecular machines, smart materials, catalysis, molecular recognition, and sensing among others² thanks to the different synthetic methodologies that had been developed over the years.³ In my talk, I will discuss a new general approach to stimuli-responsive cleavable macrocycles (e.g. chemical, photochemical, enzymatic) based on a bipyridine motif and the application of the latter in the synthesis of stimuli-responsive rotaxanes and catenanes.⁴ In addition, I will show that this platform can be applied to other macrocycles for rotaxane synthesis (e.g. crown ether) demonstrating the versatility of this chemistry.



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Information ratcheting information

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The key role of DNA is to store information.¹ In order for this to be useful, it must be possible to read that information so it can be used, for example, in DNA replication or protein synthesis. This process cannot be controlled simply through thermodynamic preferences arising from complimentary base pairing, as that would be both too slow and provide insufficient fidelity, leading to information loss.² Instead, kinetic control over selectivity is also required in addition to the thermodynamic preference. Biology realises this using sophisticated molecular machinery (DNA polymerases, ribosomes).¹ Using an information ratchet approach,² we have constructed a DNA-based reaction network which leverages structural asymmetry in the DNA strands to introduce kinetic asymmetry in the reaction network. This enables control over concentrations through differences in reaction rates under nonequilibrium conditions sustained by continuous energy dissipation from a fuel-to-waste reaction. Under nonequilibrium conditions, selectivity for the red fluorescent duplex (RT) over the green fluorescent duplex (GT) is enhanced from 2:1 up to 6:1, which is sufficient to increase the information content written upon duplex formation from 7% to 38% of the potential maximum. Though still far short of the near 100% values routinely achieved by biological systems,³ this demonstrates that the information transferred when writing on DNA (as occurs in DNA replication or protein synthesis) can be successfully enhanced using abiotic techniques. While the current work does not offer a full picture, nonetheless it has implications for the plausibility of the abiotic origin of molecules with lifelike properties.

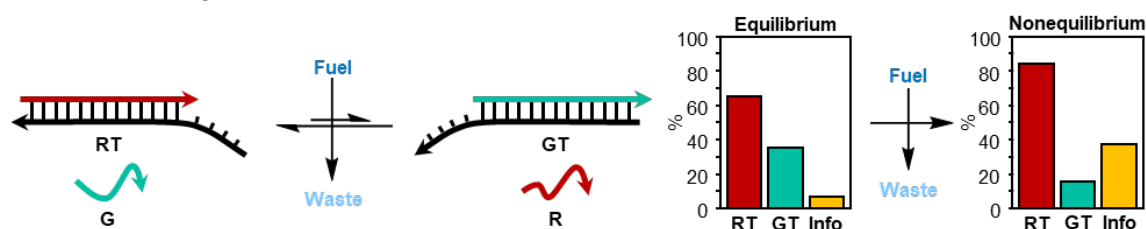


Figure 1. The exchange reaction between two fluorescent DNA duplexes can be driven away from equilibrium by coupling it with an energy-dissipating fuel-to-waste reaction. This is an information ratcheted process, analogous to autonomous chemically fuelled molecular motors. Driving the system away from equilibrium increases the amount of information written in the system from 7% to 38% of the potential maximum.

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Repurposing a catalytic cycle for transient self-assembly

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Life operates out of equilibrium to enable various sophisticated behaviors. Synthetic chemists have strived to mimic biological non-equilibrium systems in such fields as autonomous molecular machines¹ and dissipative self-assembly.² Central to these efforts has been development of new chemical reaction cycles,³⁻⁵ which drive systems out of equilibrium by conversion of chemical fuel into waste species. However, construction of reaction cycles has been challenging due to the difficulty of finding compatible reactions that constitute a cycle. Here, we realized an alternative approach of repurposing a known catalytic cycle as a chemical reaction cycle for driving dissipative self-assembly.^{6,7} This approach can overcome the compatibility problem, because all steps involved in a catalytic cycle are already known to proceed concurrently under the same conditions. Our repurposing approach is applicable to diverse combinations of catalytic cycles and systems to drive out of equilibrium, which will substantially broaden the scope of out-of-equilibrium systems.

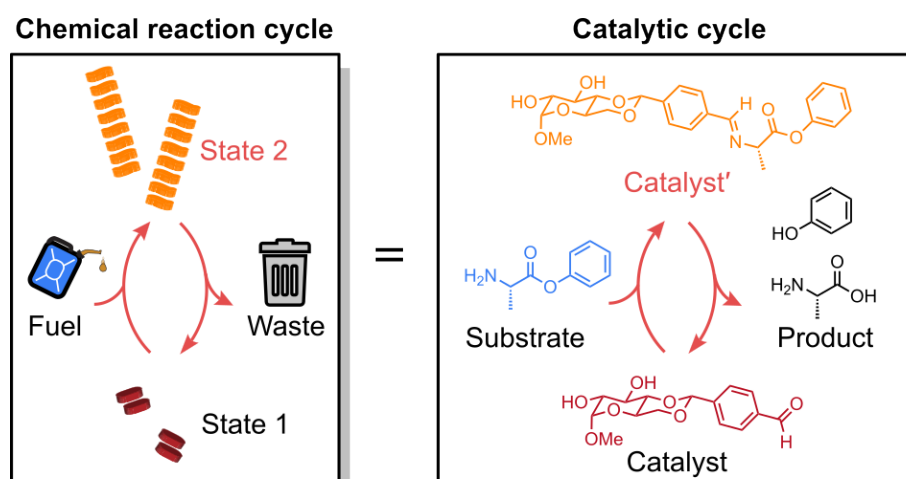


Figure 1. Repurposing of a catalytic cycle as a chemical reaction cycle for transient self-assembly.

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Out-of-Equilibrium Mechanical Disruption of β -Amyloid-Like Fibers using Light-Driven Molecular Motors

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Artificial molecular motors have the potential to generate mechanical work on their environment by producing autonomous unidirectional motions when supplied with a source of energy. However, the harnessing of this mechanical work to subsequently activate various endoenergetic processes that can be useful in materials science remains elusive. Here, it is shown that by integrating a light-driven rotary motor through hydrogen bonds in a β -amyloid-like structure forming supramolecular hydrogels, the mechanical work generated during the constant rotation of the molecular machine under UV irradiation is sufficient to disrupt the β -amyloid fibers and to trigger a gel-to-sol transition at macroscopic scale. This melting of the gel under UV irradiation occurs 25 °C below the temperature needed to melt it by solely using thermal activation. In the dark, a reversible sol–gel transition is observed as the system fully recovers its original microstructure, thus illustrating the possible access to new kinds of motorized materials that can be controlled by advanced out-of-equilibrium thermodynamics.

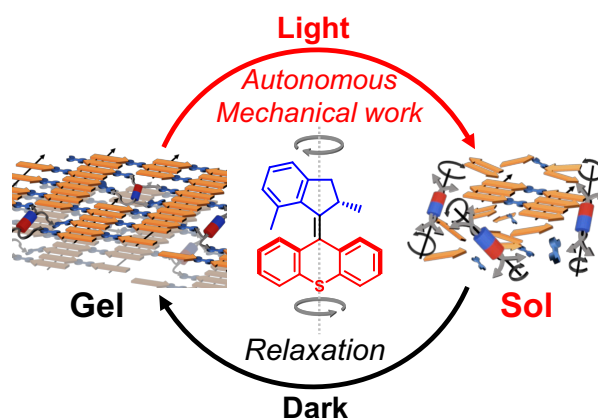


Figure 1. A light-driven rotary motor is co-self-assembled in a β -amyloid-like structure forming supramolecular hydrogels. Upon UV irradiation, the work produced by the continuous rotation of the motor is shown to disrupt the hydrogen bonds of the self-assembled system, leading to an endergonic gel-to-sol transition in out-of-equilibrium conditions. The structure of the original hydrogel is subsequently recovered in the dark..¹

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A Molecular *Primum Mobile*

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Incontrovertibly, building up intelligent supramolecular nanomaterials in a bottom-up fashion is the utmost achievement of the molecular switches and machines community. But even more appealing is the possibility of moving these materials from the bottom spheres, exerting an external control at each level, from the nanoscopic to macroscopic one, thanks to multiresponsive building blocks.^{1,2} Here we report supramolecular coordination polymers formed between metal ions and polyoxometalate hybrids bearing two terpyridine ligands in a linear geometry (Figure 1).^{3,5} Upon complexation, the polymeric chains self-assemble in fibers, on account of the electrostatic forces between the negatively charged polyoxometalate cores and the positively charged metal nodes. Eventually, the fibers physically cross-link and confer to the material a gel structure. Through SAXS and electron microscopy experiments, supported by molecular dynamics, we were able to infer the molecular-level arrangement of the polymers in the fibers. Thanks to their intrinsically dynamic nature, these gels exhibit not only interesting mechano- and thermo-responsive properties, such as birefringence or self-healing after breaking, but most interestingly the capability of yielding long-range effects by responding to minor inputs addressing the different building blocks, at the molecular, supramolecular or macromolecular level.⁶

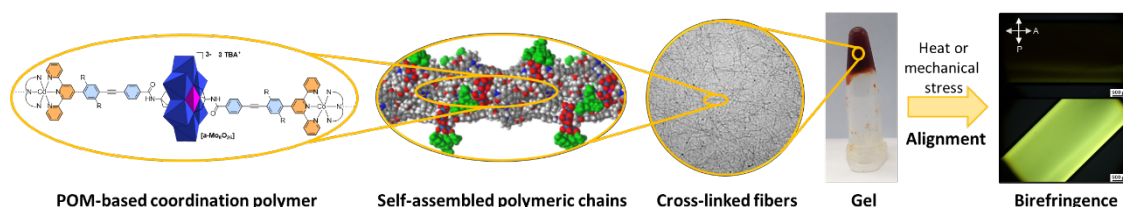


Figure 1. Self-organization from the molecular to the material level.

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Ultra-Fast Molecular Rotor Dynamics: from isolated to densely packed rotor layers

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Metal-organic frameworks (MOFs) provide a versatile platform that enables the incorporation of ligands into various structural and chemical environments, thereby fine-tuning the ligand's interactions with adjacent components within the MOF. This flexibility of MOFs allows the study of molecular rotors in diverse packing arrangements. Traditionally, achieving rapid rotary dynamics involves isolating molecular rotors, which serve as struts in MOFs, to minimise intermolecular interactions. For example, recent studies have shown that incorporating bicyclo[1.1.1]pentandioate (FTR) rotors into a cubic framework resulted in isolated rotors with a rotational energy barrier of only 6 cal/mol (Fig. 1A).¹ This low energy barrier indicates efficient rotary motion, which is essential for applications in molecular machines and sensors.

Furthermore, we inserted the dipolar FTR-F2 rotor in the Al-MOF, which forms densely packed layers of interacting rotors oriented in various configurations. Contrary to expectations, these rotors remain highly dynamic down to 4K, undergoing a cooperative reorientation cascade with a reorientation barrier of approximately 17 cal/mol (Fig. 1B).²⁻³ This discovery opens new possibilities for designing materials with dynamic properties tunable to cryogenic temperatures, which can lead towards tuning the dielectric properties of materials using densely packed orientable dipolar rotors.

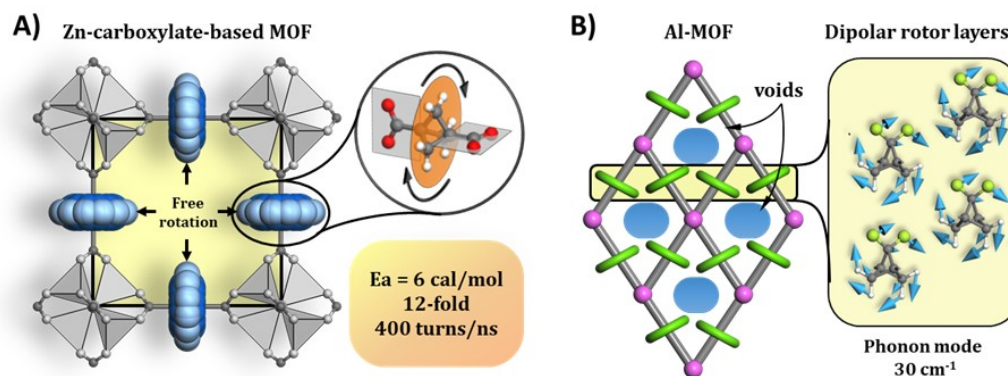


Figure 1. A) Zn-carboxylate-based MOF containing isolated (FTR) rotors (red). B) The dipolar molecular rotors in Al-FTR-F2 with dynamics down to 4 K, as shown by the ^1H relaxation rate spectrum.

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Pushing light-driven molecular motors towards perfection

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Artificial molecular motors and machines constitute a critical element in the transition from individual molecular motion to the creation of collective dynamic molecular systems and responsive materials.¹⁻² The design of artificial light-driven molecular motors operating with high efficiency and selectivity constitutes an ongoing fundamental challenge.³ Recently, we present a highly versatile synthetic approach based on Rieche formylation, which boosts the quantum yield of the forward photoisomerization reaction while reaching near-perfect selectivity in the steps involved in the unidirectional rotary cycle and drastically reducing competing photoreactions.⁴ This strategy not only provides a general approach to make high performance all generation molecular motors that operates with nearly quantitative photoconversions, but also leaves opportunities for transforming functionalities.^{5,6} This versatile design of the light-driven molecular motors show huge potential for their dynamic applications.

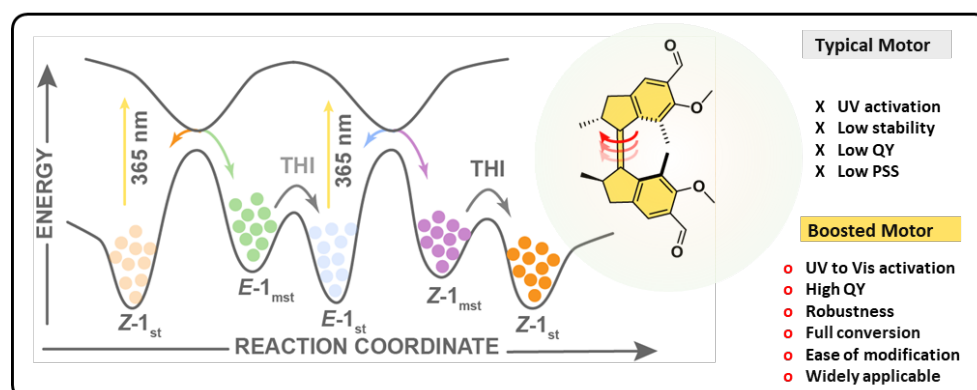


Figure 1. Conceptual illustration of rotary motion of boosted molecular motors system. The boosted motor structure presented here, along with schematic depiction of the corresponding potential energy surfaces of the rotation cycle of the boosted molecular motor, with a common quantitative photochemical E–Z isomerization step followed by an irreversible and quantitative THI step. The light and dark shading in the orange and blue circles shows how many motors will be converted into next state. The right panel compares the characteristics of typical and boosted molecular motor systems.

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Shining Light on Porous Solids

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Nature has developed an intricate array of molecular machinery that powers nearly all aspects of metabolism, from protein synthesis to both cellular and macroscopic movement. These molecules, usually proteins or multi-protein complexes, typically operate while immobilized, a necessary condition to harness their work amid overwhelming thermal noise. Inspired by this complexity and versatility, a plethora of small molecule artificial molecular machines and switches have been designed and synthesized.[1] Yet most of these synthetic counterparts have primarily been designed and studied in diluted solutions, where the overwhelming Brownian motion precludes any cooperative action. Therefore, development of practical strategies enabling spatial immobilization and organization of these dynamic small molecules as well as synchronization of their work remains a fundamental challenge.[2]

This talk will summarize our research on integrating artificial molecular machines and switches into extended porous frameworks. This approach not only facilitates the organization and immobilization of these functional molecules but also allows us to harness their collective motion within the material scaffold.[3,4] Our exploration covers a range of structures: beginning with rigid frameworks where molecular motion is restricted to individual molecules[5,6] and progressing to amorphous, flexible scaffolds that dynamically reorganize upon the isomerization of incorporated photoswitches.[7,8] Beyond these simple systems we venture into more complex architectures where multiple responsive units can operate independently, thus further extending the potential of these structures to exhibit intricate and adaptive behaviors.[9]

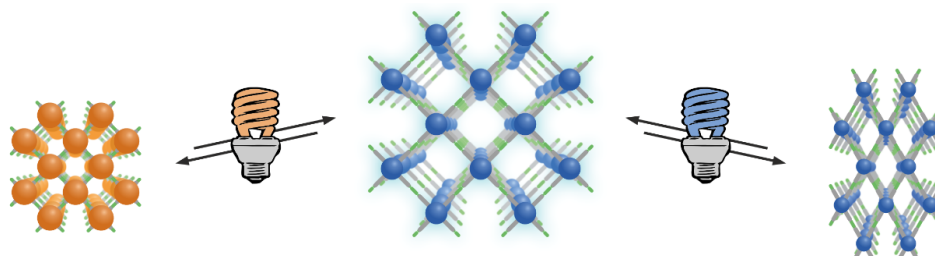


Figure 1. Cartoon depiction of photoswitching within a porous framework

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Triplet-Sensitized Isomerization of Azoswitches

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Triplet-sensitized isomerization emerged as a powerful tool in the photoswitching field. This indirect photoswitching approach leaves the intrinsic properties (such as long half-life) of photoswitches but expands the excitation modality beyond its capabilities by introducing a proxy system responsible for harvesting the excitation of longer wavelengths and transferring this energy to the photoswitch. Previously our group has shown that conventional azobenzenes can undergo indirect $Z \rightarrow E$ photoisomerization via triplet sensitization even upon 770 nm light excitation of a sensitizer (instead of e.g. green one).¹ Recently, encapsulation of triplet sensitizers and different azobenzenes into a supramolecular cage allowed to perform $E \rightarrow Z$ photoswitching upon red 640 nm light illumination of a sensitizer.² Intrigued with this photoswitching “under confinement” phenomenon, we turned our attention to azobenzenes that are already chemically constrained i.e. diazocines. In striking contrast to azobenzenes, diazocine can be selectively switched in $E \rightarrow Z$ direction and most intriguingly from its thermodynamically stable Z to metastable E isomer upon successive excitation of two different triplet sensitizers present in plain solution at the same time. Moreover, this approach leads to an extraordinarily large redshift of excitation wavelengths to perform isomerization i.e. from 400 nm blue to 530 nm green light ($Z \rightarrow E$) and from 530 nm green to 740 nm far-red one ($E \rightarrow Z$).³

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A Hemithioindigo Molecular Motor Operating by Constitutional Alteration and Hydrogen Bonding

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Molecular motors provide repetitive unidirectional motions by harvesting energy and they have become an essential component in miniaturized future machinery. The autonomous behavior of a molecular motor results from different sources of energy, yet light is able to induce large and well-defined structural changes in a fast, “economic” and “green” manner.^[1] Over the past two decades, three main class of compounds have been explored for light-induced double bond isomerization: overcrowded alkenes,^[2] imines,^[3] and hemithioindigos.^[4] While hemithioindigo-based photochromic molecules present some structural features similar to overcrowded alkenes, they are exclusively driven by non-destructive visible light and enable fast directional motions at room temperature.^[5] Despite the great progress in synthetic molecular machines, hitherto artificial systems still cannot reach the outstanding capacity and complexity of their biological congeners in terms of operation or functionality. Development of new molecular motor setups and using their unidirectional motions to accomplish energetically uphill processes thus lie at the current forefront of molecular machinery research. In this communication, an unprecedented and highly efficient mechanism for light-driven motor rotation will be showcased.^[6] Unlike earlier molecular motors, the herein described hemithioindigo derivative exploits constitutional alteration and subsequent hydrogen bonding to complete its fully unidirectional motion rather than steric effects. This unique rotational mechanism also stores substantial amount of light energy and opens up new avenues for next generation of molecular machines with enhanced action and power.

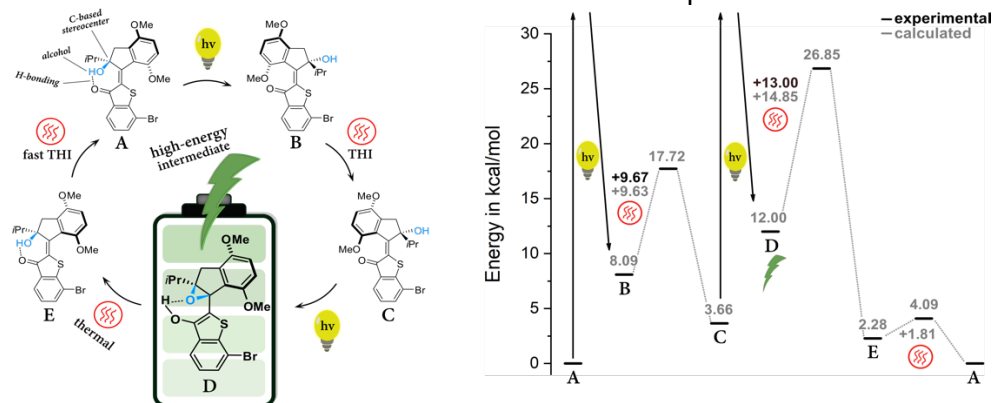


Figure 1. Rotational cycle of hemithioindigo-based molecular motor operating via constitutional alteration and hydrogen bonding.

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Coupling Rotary Motion to Helicene Inversion within Molecular Motors

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An overcrowded alkene-based molecular motor comprising an extended dibenzo[c,g]fluorene moiety has been previously synthesized and studied by our group.¹ This compound displays a bathochromic shift of the excitation wavelength allowing for visible-light driving of the rotation. DFT calculations showed that each step in the rotary cycle induced an inversion of the helicity of the dibenzo[c,g]fluorene, giving rise to a coupled paddling motion along with the rotation of the motor.² This phenomenon could unfortunately not be studied experimentally due to the very low racemization barrier of the dibenzo[c,g]fluorene lower part. Such coupled motions are unusual phenomena of high interest for the design of new molecular systems displaying higher levels of functionality³ and open the way to a range of new applications. We now aim at controlling this paddling motion by tuning the racemization barrier of the lower half, allowing to study this phenomenon and use it for applications ranging from new helicity driven molecular motors to chiroptical switches performing remote helicity inversions upon photoactuation. The newly developed compounds, associated synthetic routes and photophysical studies will be presented.

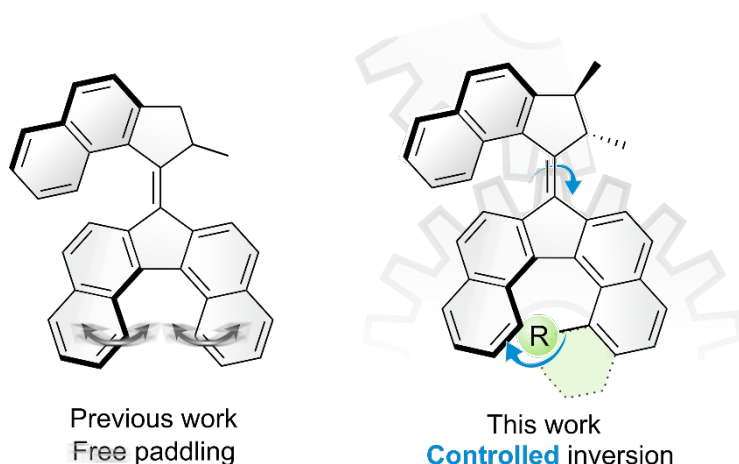


Figure 1. Second-generation molecular motors featuring an helical dibenzofluorene bottom-half.

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Photoluminescence for Molecular Machines and Devices

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After the successful development of light-driven molecular motors in the past decades, the next challenge is to combine the unidirectional rotary motion of these nano-machines with other light-mediated functions. Especially, photoluminescence (PL) properties are expected in terms of single-molecule imaging and development of photoswitchable devices. A PL dye and a molecular machine are combined in a single molecule¹ and in a liquid crystal device,² resulting in synergistic photofunctions and programmed modulation of circularly polarized light emission (Figure 1).

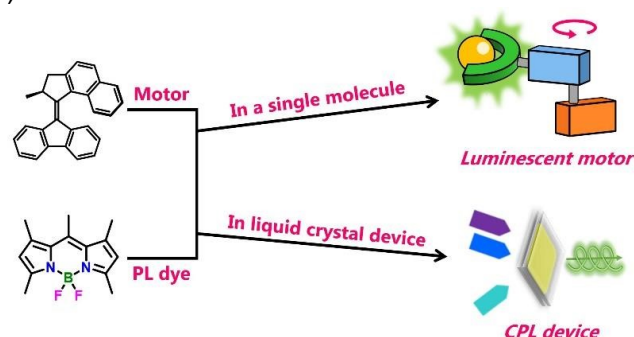


Figure 1. Combination of a PL dye and a molecular motor.

Also, PL can play a pivotal role in molecular devices. For miniaturization of devices, photons rather than electrons are expected to be utilized to convey information or energy. A series of molecular nanowires are fabricated by connecting photoluminescent dyes using coordination chemistry techniques.³⁻⁵ Our theoretical modeling making use of the well-defined molecular structures successfully elucidated the dynamics of exciton transfer within the molecular chains (Figure 2).

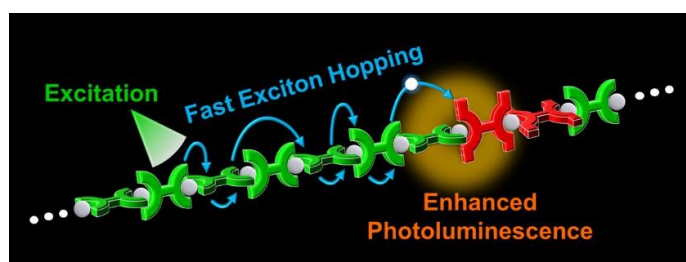


Figure 2. Exciton migration within a molecular nanowire.

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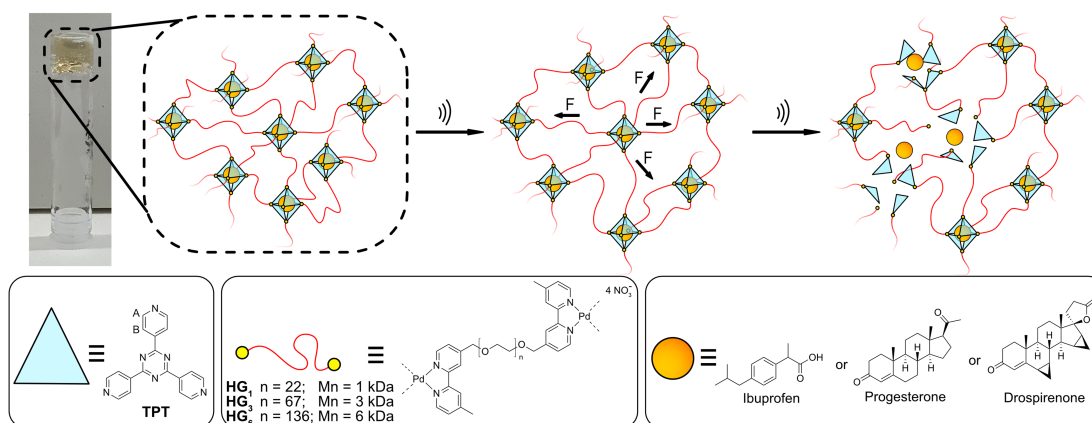
Mechanoresponsive Metal-Organic Cages

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My research group is involved in various aspects of supramolecular chemistry, including our pioneering work in the field of mechanoresponsive supramolecular systems, which we could use for the release of non-covalently bound guests from an aqueous solution.

The mechanochemical release of cargo molecules from their respective latent carrier polymers is challenging.¹ We published a versatile system based on a supramolecular coordination cage as complex mechanophore in 2021. By combining metal-mediated self-assembly of organic ligands into a discrete nanoscopic structure with polymer chains on each vertex, we realised the ultrasound-induced disassembly of a cargo-loaded, self-assembled supramolecular Pd^{II}₆(TPT)₄ cage, entailing the release of its nanoconfined guests. This is exemplarily demonstrated for several non-covalently bound, completely unmodified, but pharmaceutically active compounds.² In addition, we now report bifunctionalized byridines that can be used to generate metal-organic cage-based hydrogels, combining supramolecular chemistry with soft matter.³



The encapsulation of guest molecules into supramolecular self-assembled metal-organic cage-crosslinked hydrogels, as well as ultrasound-induced disassembly of the cages with release of their cargo, is presented in addition to their characterization by rheology and small-angle X-ray scattering (SAXS) experiments. The constrained geometries simulating external force (CoGEF) method and barriers using a force-modified potential energy surface (FMPES) suggest that the cage-opening mechanism starts with the dissociation of one pyridine ligand at around 0.5 nN.

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Tuning Biocolloidal Taxis and Catalysis in Gradient of (Oilgo)nucleotides

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Biology used external stimuli to regulate feedback loops and modulate enzymatic reactions within cells both as a function of time and space.¹ Therefore, incorporating catalysis along with functions like – adaptability, stimuli responsiveness, dynamic specificity towards certain receptors or reactions and precise spatial and temporal control can make a synthetic system much closer to complex natural processes. To develop such systems, a catalyst must autonomously be relocated in different zone and toggled between on/off state. Importantly, gaining control over this process will be crucial for the development of spatially segregated chemistry to synthesize novel products or complex structures that are not accessible using conventional methods. Herein, we addressed the above-mentioned issue by modulating phoretic behaviour of colloids through temporally altering multivalent interactivity with nucleotides. Importantly, the catalytic property of the colloid can be autonomously controlled in a temporal fashion by the convertible multivalent scaffold around it. Therefore, multivalent interactivity can control both the phoretic motion of the colloid to dictate spatial location and the temporal control over catalytic process. Multivalency mediated interaction coupled with catalysis plays crucial role in regulating several dynamic self-assembly processes inside living systems, like microtubule dynamics, growth and contraction of actin filaments etc. Despite its significance in supramolecular material chemistry to biomedicine, the potential of such systems in modulating colloidal phoresis or motion and catalytic properties and thereby understanding of precise spatial behavior remains unexplored.

Herein, we realize and control previously mentioned life-like behaviours in a synthetic system by tailoring multivalent interactions of adenosine nucleotides and catalytic microbead.^{2,3} The research results can find applications - in programming the delivery of colloids for chemical processes (e.g. catalysis or drug release) as a function of space and time by switching on or off phoretic activity. Moreover, these active catalysts can function as sensors in far-off places because they don't need any external power sources.

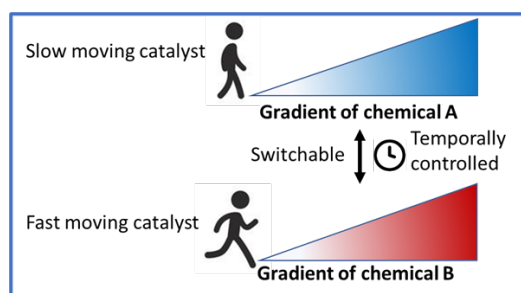


Figure 1. Schematically showing the theme of the system where directional motion of the catalyst (a micron-sized bead) can be modulated in different chemical gradients. In our case, we found catalyst moves slowly in gradient of ATP, however in a gradient of ATP hydrolyzed products (AMP + 2Pi) it moves faster, thereby spatial control over catalysis can be achieved by modulating ATP-hydrolysis rate.

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Controlled fusion of polymer nanoparticles

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Encapsulation of cargos into vesicle containers is key for the controlled movement of material around and between biological cells. This organized compartmentalization of biological cargos is essential for many processes, such as protein modification, nerve signalling and immune response coordination.¹ The ability to reproduce such a 'parcel delivery surface' using abiotic containers would allow control over the mixing of molecular cargos in a synthetic setting, providing new methods to control chemical reactivity at the nanoscale. Here we present the first step to realizing such a system. Kinetically trapped polymer nanoparticles² capable of undergoing fusion on demand can be accessed by ring-opening metathesis polymerization-induced self-assembly (ROMPISA).³ These particles relax by fusing together to give elongated tubular nano-objects. By tuning vesicle surface charge and membrane tension, it is possible to trigger fusion by a pH switch.⁴ Furthermore, the crossed fusion of two different nanoparticle populations is possible by adjusting corona chemistry and membrane tension. The nanoparticles have been characterized by various methods, including cryo-TEM and *in-situ* SAXS. Complex cascades of fusion are currently under investigation.

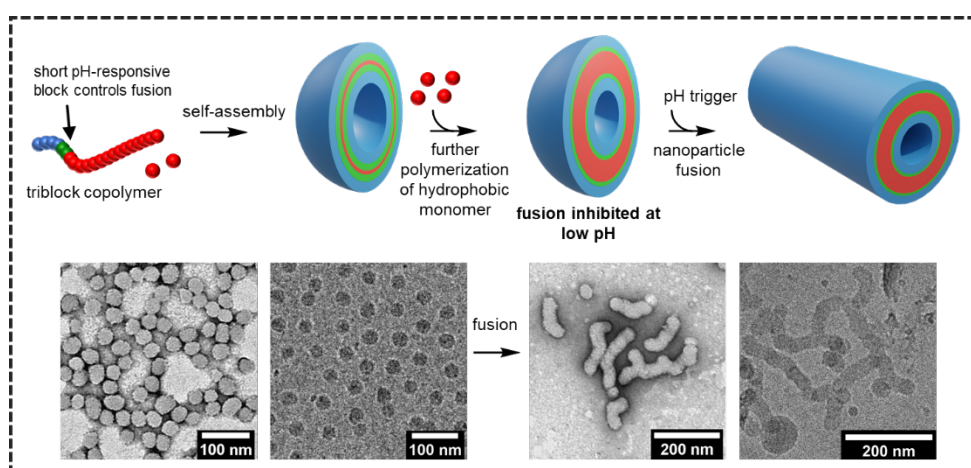


Figure 1. Design and TEM images of controlled polymersome fusion process.

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Molecular Motors Driven by Electrons and Protons

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Molecular motors in biological systems have inspired attempts to create artificial molecular machines¹ that can produce controlled motion on the molecular level. My talk will describe the progress we have made towards the design and synthesis of a four-stroke rotary motor based on a [3]catenane which contains cyclobis(paraquat-*p*-phenylene) (CBPQT⁴⁺) and dibenzo-[24]crown-8 (DB24C8) as two rotors and a loop passing through them as a stator. The loop contains in sequence four stations which are a viologen dication (V²⁺), a dibenzylammonium cation (DBA⁺), a 1,5-dioxynaphthalene (DNP) unit and a methyltriazolium cation (MTA⁺). The DNP and V²⁺ can act² as different binding sites for CBPQT⁴⁺ / CBPQT²⁽⁺⁾ under different redox conditions and DB24C8 can switch^{3,4} between the DBA⁺/DBA and MTA⁺ units under different pH conditions. By changing the redox and pH conditions alternatively, the CBPQT⁴⁺ / CBPQT²⁽⁺⁾ and DB24C8 rings can move clockwise or anticlockwise on the track and “stop” on one of the four stations. This investigation will promote an efficiency artificial molecular machine that driven by electrons and protons.

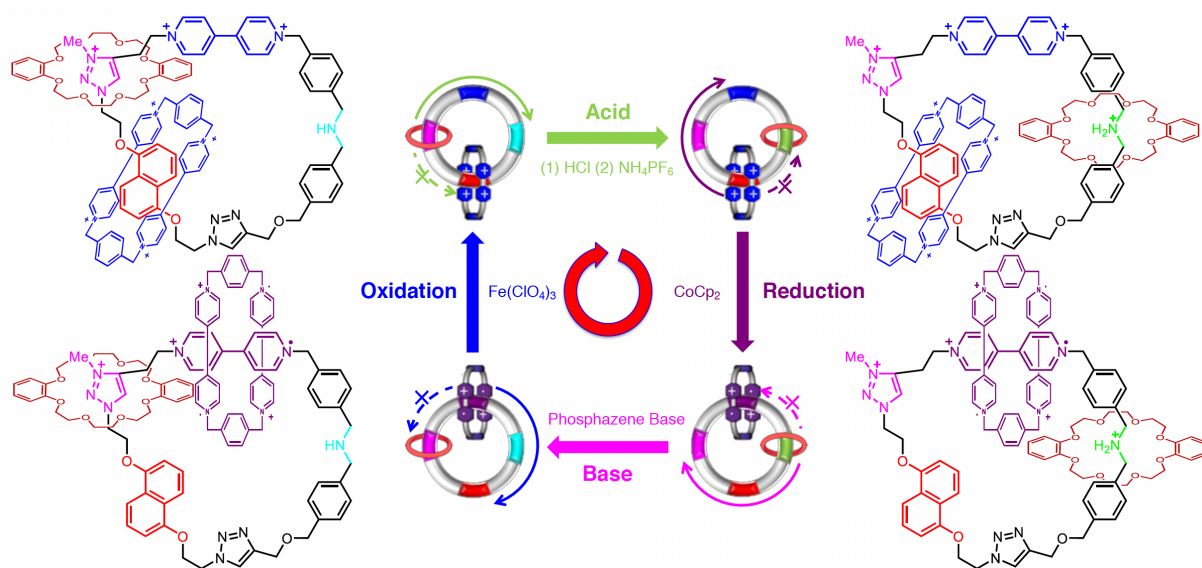


Figure 1. Graphical representations and the structural formulas of the four-stroke unidirectional rotary cycle controlled by the redox and pH stimuli.

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Light-driven ratcheted self-assembly of diastereomeric host-guest systems

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The use of an energy source to drive chemical reactions away from equilibrium is essential for life and a major challenge in designing fuel-powered artificial nanosystems.¹ In this study, we examine how light irradiation affects the self-assembly of supramolecular complexes made of azobenzene-type guests and a cyclodextrin (CD) host in water. Unlike previous studies that focused on equilibrium properties, our research investigates the distributions far from equilibrium achieved through light-driven self-assembly. We demonstrate that photoirradiation can invert the relative abundance of the two CD orientational diastereomeric complexes and showcase a ratcheted approach² to the self-assembly of high-energy CD complexes in an aqueous environment, utilizing biocompatible macrocycles and visible light (Figure 1). This strategy holds potential for developing active materials, designing artificial metabolic networks, and engineering molecular machines that function in physiological conditions.

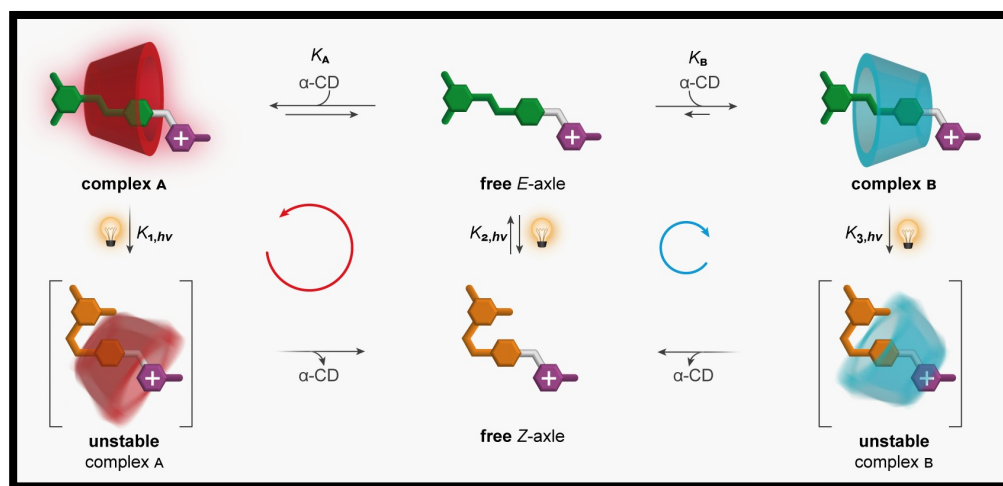


Figure 1. Light-driven self-assembly of the two CD orientational diastereomeric complexes.

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Modulation of Mechanical and Nanostructural Properties of a pH-Responsive Self-Assembled Hydrogel

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Peptide-based self-assembled hydrogels have a wide range of biomedical applications thanks to their mechanical properties and good cytocompatibility. An added value is the nanomorphological diversity resulting from their self-assembly, such as nanofibers, nanowires, or nanotubes, with useful properties in drug delivery, biosensing, or the development of semiconductors.¹ Due to the synthetic accessibility and dynamic nature of peptide self-assembly, the introduction of molecular switches (**MSs**) within their structures (pH-, photo-, or redox-**MSs**) emerges as a useful strategy for the development of smart materials.²

In this study, we present a new pH-responsive hydrogelator **V-FfFH₂·2Cl** (Figure 1), comprising the so-called “vermellogen” motif (**VH²⁺**)³ and a hydrophobic heterochiral sequence (L-Phe-D-Phe-L-Phe, **FfFH**). **V-FfFH₂·2Cl** exhibits two ionizable groups in solutions ($pK_a^1 = 3.3$, $pK_a^2 = 9$), allowing its amphiphilic character to be tuned by varying its net charge with pH. This pH-responsiveness of **V-FfFH₂·2Cl** is transferred from the molecular scale to the nanoscale, and all the way up to the macroscale, forming pH-tunable hydrogels with variable mechanical properties and nanostructures.

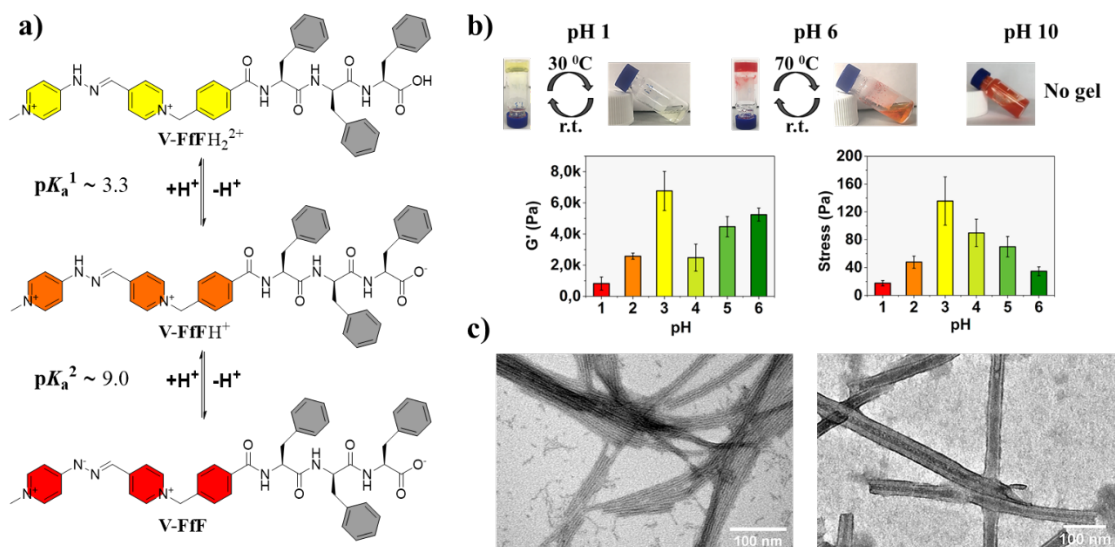


Figure 1. a) Schematic depiction of the **V-FfFH₂·2Cl** structure with the corresponding acid-base equilibria. b) Photographs of the self-assembled hydrogels and viscoelastic properties at different pHs. c) TEM images of the hydrogels at pH1 (left) and pH6 (right), showing an evolving nanotube size.

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Design and characterization of complex reaction networks in dynamic mechanically interlocked molecules

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Mechanically interlocked molecules (MIMs) have been extensively exploited for the development of artificial molecular machines (AMMs), as the application of various chemical stimuli (e.g., redox, light, or pH) can induce co-conformational modification resulting in mechanical-like movements.¹ The characterization of the complex reaction networks underlying the AMMs² represents the common thread linking the projects here discussed.

The first example focuses on the investigation of a [3]rotaxane in which a chemical property, such as the acidity of a specific site, can be modulated upon switching of the co-conformation (Figure 1a).³ This behavior is analogous to allosteric effects observed in biomacromolecules. In a second example, a photoinduced proton transfer within [2]rotaxanes is exploited to trigger the movement of a macrocycle across two recognition sites, representing a novel strategy to induce a light-driven shuttling motion (Figure 1b).⁴

The final example involves a photoactive molecular pump that uses photochemical and self-assembly reactions to harvest light energy, driving the threading of macrocycles from the solution to a linear molecular reservoir (Figure 1c).

Beyond the fundamental interest, the understanding of the kinetic and thermodynamic aspects underlying AMMs operation is crucial for the improvement of their performance thus opening new perspectives for innovative applications in nanotechnology.

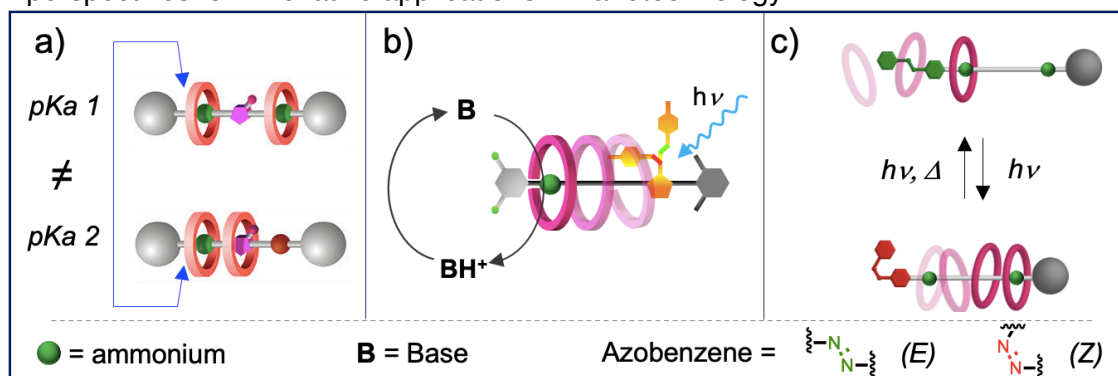


Figure 1. Graphical representation of the AMMs discussed.

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Beyond Acid-Base Reactions: Interfacing Activated Carboxylic Acids with Electrical Circuits

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Upon deprotonation by an appropriate base catalyst, Activated Carboxylic Acids (ACAs) irreversibly liberate CO₂ and are therefore converted into strong carbanionic bases that take back the proton, as shown in Figure 1.¹ Thanks to their ability to transiently alter the acidity of their environment, ACAs have found application in the programmable operation of acid-base-sensitive systems, allowing the control of the movement of molecular machines,^{2,3} the regulation of catalysis,⁴ or the translocation of metal ions.^{5,6}

In aqueous solutions, ACAs can be used to temporally control the pH going from high pH (before the acid addition) to low pH (upon acid addition), and back to high pH (after decarboxylation of the ACA and proton reuptake by the carbanion base).^{7,8}

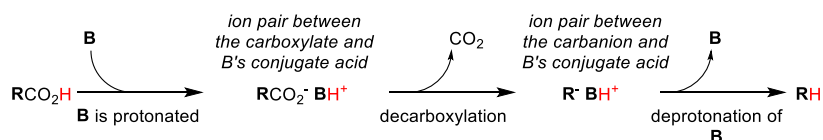


Figure 1. Working cycle of a generic ACA (RCO_2H) in the presence of an appropriate base catalyst (B).

Our work focuses on interfacing ACAs with electrical systems normally unaffected by acidity changes. Specifically, we employ ACAs to transduce a pH cycle into a voltage cycle by means of a p-benzoquinone/hydroquinone electrochemical cell. The output voltage of the cell can be used to trigger external electrical circuits.⁹ Furthermore, we turn an aqueous solution into a programmable, variable resistor by employing pulses of an ACA to transiently control its conductivity.

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Promising Diazocine Compounds for Hybrid Smart Materials

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Materials, whose properties can be changed in a controllable way by external stimuli, are known as smart materials. Especially light as an external stimulus is a harmless, well adjustable and inexpensive trigger for chemical reactions with excellent time and local resolution. Diazocine compounds are stiff photoswitches with excellent photophysical properties, which undergo *Z/E* isomerisation by changing their molecular geometry upon irradiation with visible light. Although the application of diazocines in polymers is a highly potential field of photoswitchable actuators, only a few examples have been realised by now.

Addressing the lack of suitable compounds, we report the synthesis of two novel classes of promising diazocines with improved molecular characteristics for the application in photochromic copolymers.^{1,2} Bistriphenylene diazocines exhibit several binding sites, which ensure an even stronger connection to the polymer matrix (Figure 1, left). During isomerisation, these compounds show a great amplitude of motion, which can be effectively translated into a macroscopic movement of the material in which they are integrated. Bisimide diazocines are easily accessible starting from the corresponding bisanhydride diazocines, which make them suitable components for photoswitchable polyimides (Figure 1, right). Within the polymer backbone, the substitution pattern of the diazocine goes along the horizontal molecular axis leading to an ideal power transmission for the twisting of the polymer strand.

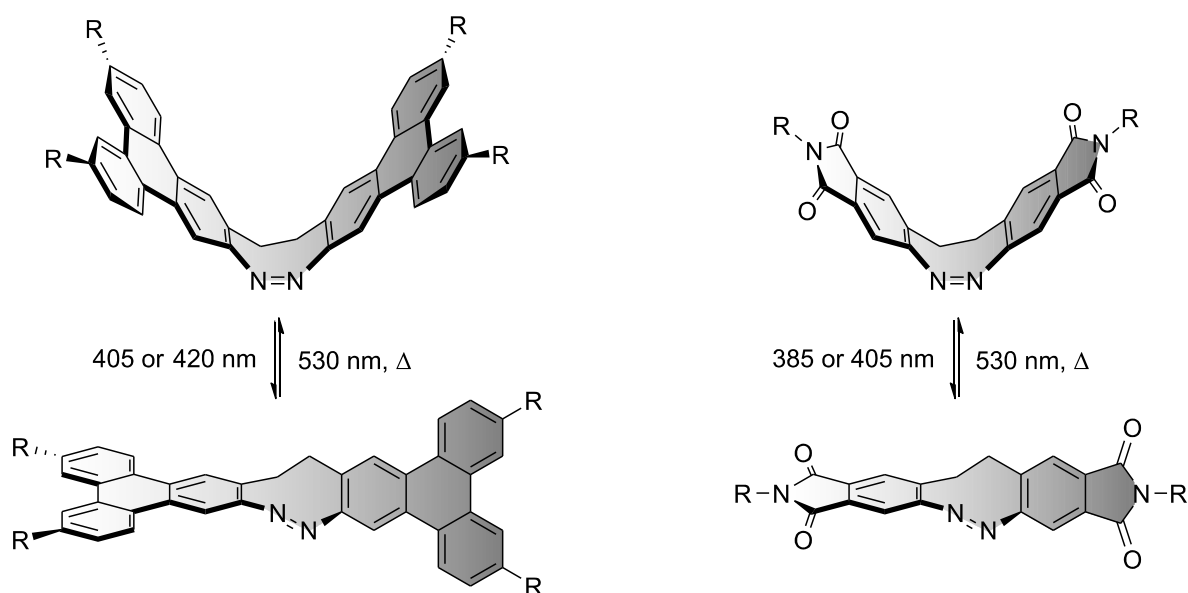


Figure 1. Light-induced *Z/E* isomerisation of bistriphenylene diazocine (left) and bisimide diazocine (right), R = polymer strands.

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Novel prototypes of multistable [2]- and [3]rotaxanes

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Rotaxanes are the most explored class of mechanically interlocked molecules (MIM), and two-stations rotaxanes are the most common architecture adopted to design artificial molecular machines.¹ Rotaxanes with a higher number of stations and rings are more sophisticated systems, in which complex operations can be performed.² We report the investigation of a family of three-stations [2]- and [3]rotaxanes, performed by voltammetric methods, NMR and UV-Vis spectroscopy. The rotaxanes are composed by one or two crown ether macrocycles and an axle comprising an ammonium primary station, a bipyridinium secondary station and a triazolium tertiary station (Figure 1). The primary and the secondary stations can be de-activated by means of orthogonal stimuli: the ammonium site can be switched-off by deprotonation (*chemical stimulus*), while the bipyridinium site by reduction (*electrochemical stimulus*). Both processes are reversible and a combination of chemical and electrochemical stimuli can be used to control the motion of the ring from one station to the other. The [2]rotaxane can be switched between three stable states (Figure 1a), in which the ring sequentially moves on the axle from one extremity to the other. In the [3]rotaxane, five different states can be accessed (Figure 1b): the two rings can reside on neighboring stations (State I and IV), on stations at the opposite extremities of the axle (State II) or on the same station (State III and V).

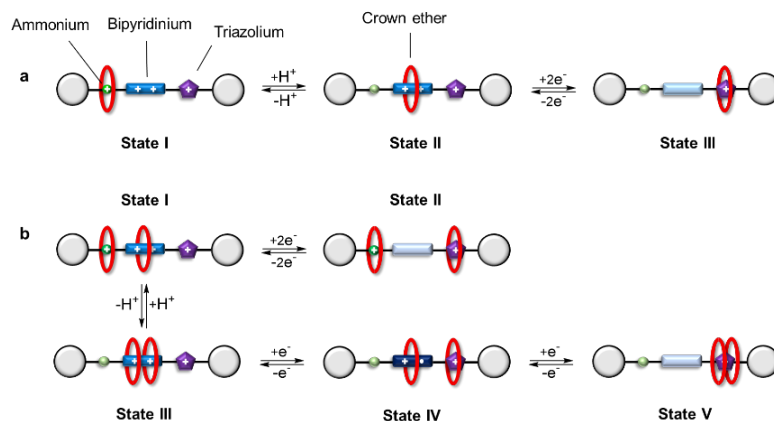


Figure 1. Schematic representation of the operation in the [2]rotaxane (a) and the [3]rotaxane (b).

A key property of these systems is the modularity: in the [3]rotaxane, the presence of an extra ring leads to a complex behavior, which retains the characteristics observed for the [2]rotaxane. This feature enables the design of novel MIMs based on the same molecular components, capable of exploiting the high degree of control over the motion of the ring to perform work. This work was supported by the European Union's Horizon 2020 research and innovation program (FET-OPEN “Magnify” 801378).

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Molecular information ratchets exploiting the asymmetry of functionalized cyclodextrins for autonomous active transport

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Information ratchets¹ are a general class of mechanism in which an energy barrier is regulated on a potential energy surface in order to drive directionally the Brownian particle distribution away from equilibrium. Creating a molecular Brownian ratchet is crucial to attain unidirectional movement in molecular machines². Cyclodextrins³ are good candidates to enhance the kinetic asymmetric because of their asymmetric conical shape⁴. Nevertheless, the kinetic asymmetric of the system could be increased even more by the regioselective functionalization on one of the faces of cyclodextrins.

Herein, we describe a bis-dimethylamine permethylated cyclodextrin [2]rotaxane which can perform autonomous active transport under addition of chemical fuels. The [2]rotaxane is composed of three equivalent spacers separated by two secondary amines as the reactive sites that can react with Fmoc derivatives. During the Fmoc-protection a kinetic bias resulting in a non-statistical distribution between the three possible mechanoisomers was observed. The spontaneous orientational mechanospecific Fmoc deprotection can be initiated by the dimethylamine arm located on the primary face of the cyclodextrin. Thus, one pure mechanoisomer can be obtained autonomously by adding continually Fmoc derivatives and base starting from a mixture of three mechanoisomers.

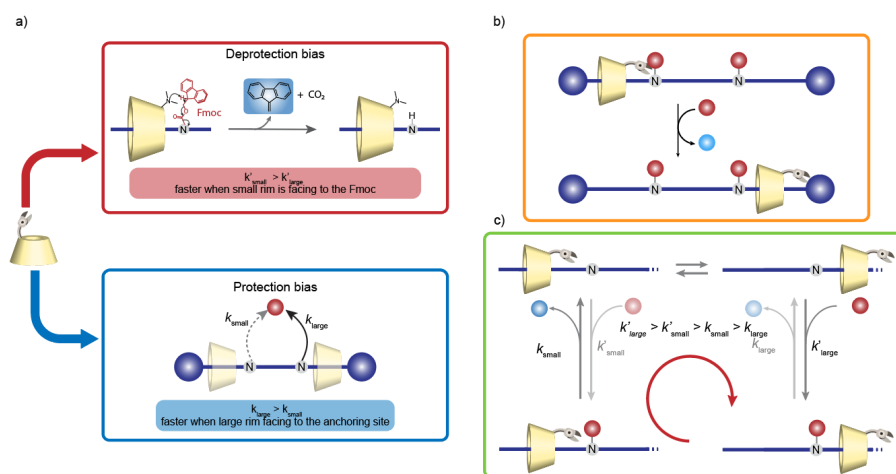


Figure 1. Kinetic asymmetric induced by the cone-shape cyclodextrin and face selective functionalization to perform unidirectional linear active transport upon addition of chemical fuel; a) kinetic biases exist during Fmoc protection and deprotection; b) active transport performed on a [2]rotaxane; c) mechanism insight of the unidirectionality.

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The Hitchhiker's Guide to Mechanical Stereochemistry

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Upon mechanical bond formation, achiral sub-components can be desymmetrised to yield chiral and geometric isomers.¹ When considering the catenation of oriented and/or facially dissymmetric macrocycles (**I** and **II**) and rotaxane formation using the same with bilaterally symmetric axles (**III** and **IV**), seven distinct isomeric motifs can be formed (**V-XI**).^{2,3} Of these, only mechanically planar chiral systems (**V** and **VIII**) have been studied significantly and axially chiral rotaxanes **XI** were only discovered in 2022.⁴ Here we report a study of the factors controlling the selective synthesis of both of geometric and chiral mechanical isomers and the first direct enantioselective synthesis of a mechanically axially chiral rotaxane. All of the fundamental mechanical stereoisomers can now be synthesised stereoselectively.^{5,6}

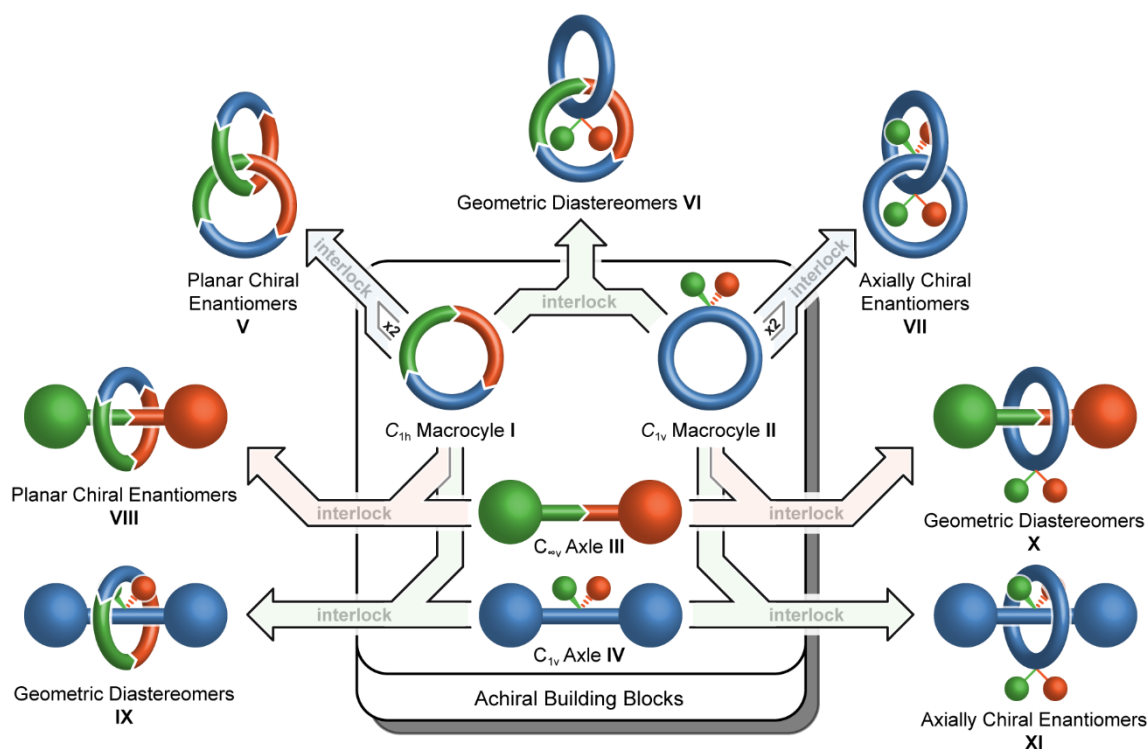


Figure 1. Mechanical isomers of [2]catenanes and [2]rotaxanes through combination of oriented or facially dissymmetric macrocycles **I** and **II** and bilaterally symmetric axles **III** and **IV**.

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Operation of Artificial Molecular Pumps in Water

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Water, as a solvent, plays a crucial role in stabilizing biological structures, mediating biochemical reactions, and facilitating molecular interactions through its unique properties such as high polarity and hydrogen bonding. These characteristics enable the precise folding of proteins and the formation of lipid bilayers, underscoring the necessity for the development of artificial systems which operate in water in order to better understand the complexities of biochemistry.

In contrast, artificial molecular machines (AMMs) which operate in water are exceptionally rare. For AMMs to achieve their full potential in mimicking biological systems, it is imperative to overcome their limited ability to function in aqueous environments. Unlike many of the forces which have been demonstrated to drive the operation of AMMs, the radical-radical interactions that power numerous^{1, 2} artificial molecular pumps (AMPs) are enhanced in water. The polarity of water effectively screens the positive charges of the viologen units, thereby attenuating the Coulombic repulsion between them and favouring their assembly. Consequently, it is reasonable to anticipate that viologen-based pumps will operate effectively in water. Despite this promising prospect, no AMPs have been demonstrated in water. While the theoretical conversion of conventional AMPs to function in aqueous environments appears straightforward, practical challenges must be addressed and overcome.

Herein, we report the design of an artificial molecular pump and the development of protocols for its operation in water. The operation of this AMP in water exhibits improved kinetics and efficiency compared to pumping in organic solvents, thereby efficiently producing [2] and [3]rotaxanes.

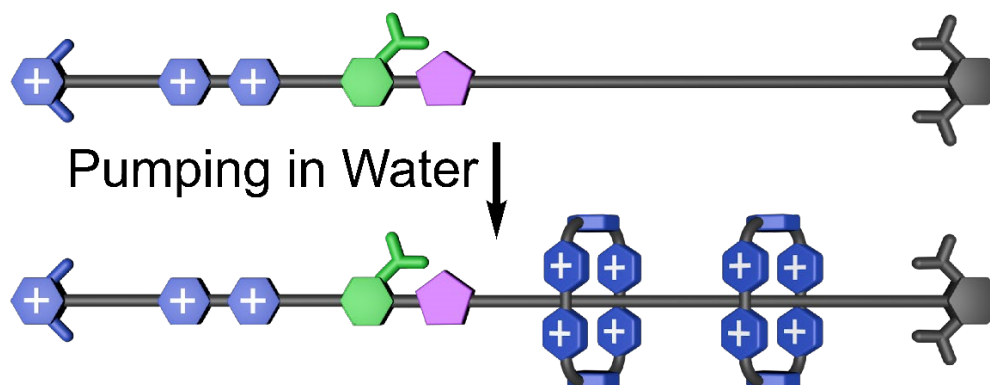


Figure 1. Graphic depiction of the formation of [2] and [3]rotaxane by pumping in water.

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Influence of geometrical photoisomerization in dynamic self-assembly

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Abstract The ability of a dynamic self-assembled structure to adapt to environmental changes is a fundamental and desirable property for chemical systems, particularly in the development of complex matter and life-like materials.¹ Here, we successfully navigate between two self-assembly orders (a molecular cage and macrocycles) using light as an external stimulus. This is achieved by exploiting the capability of a photoswitchable building block to govern the state of self-assembly.² When different complementary building blocks are present, the state of the switch determines the predominant architecture, adapting the self-assembly to form either a cage or a macrocycle. This yields a diverse collection of reversible cage-to-macrocycle transformations with constitutional dynamic adaptation of the self-assembled structure and the building blocks in the solution. Our study showcases this principle with eight different examples of light-fueled cage-to-macrocycle transformations, offering an unprecedented level of diversification and adaptability.

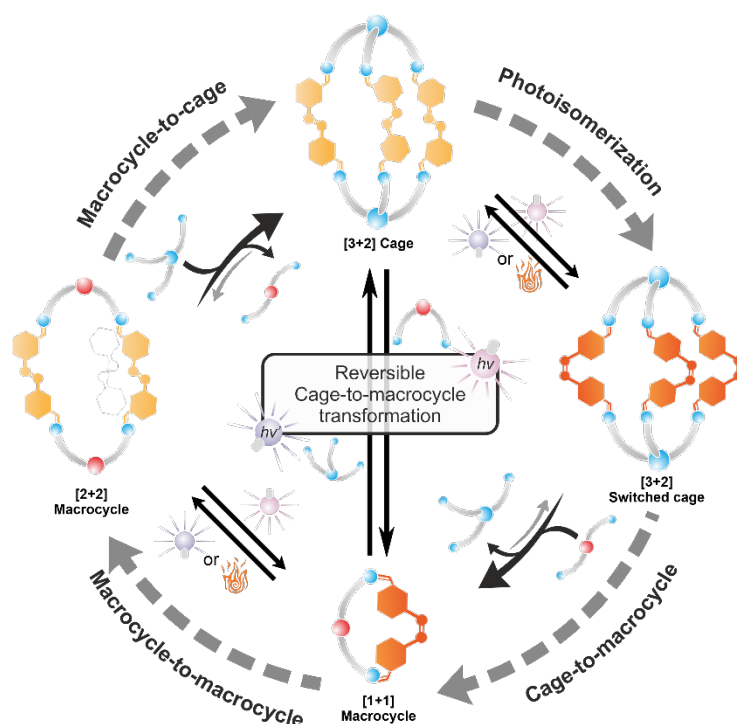


Figure 1. Different self-assemblies governed by a photoswitchable building block. **Photoisomerization** of a [3+2] cage occurs reversibly upon an external stimulus. When a ditopic complementary building block is present, the isomerized cage undergoes a [3+2]cage-to-[1+1]macrocycle transformation. When isolated, the [1+1]macrocycle-to-[2+2]macrocycle transformation can be controlled with a photochemical stimuli. In the presence of a competing tritopic complementary building block, the [2+2]macrocycle-to-[3+2]cage transformation occurs. When all the components coexist in solution, a reversible [3+2]cage-to-[2+2]macrocycle is controlled with light.

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Wavelength-steered motion in an autonomous light-driven molecular rotor

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By combining photophysical and photochemical reactivity with appropriately designed molecular systems, it is possible to realize nanoscale devices and machines that can execute sophisticated tasks in response to light stimulation. In particular over the past two decades, there has been significant research focused on rotary motors based on stilbene,¹ imine,² hemithioindigo,³ and related structures. Nonetheless, all the reported artificial light-driven molecular rotors present intrinsic limitations related to their synthetic accessibility, stability or efficiency of operation, that altogether hinder their broad application.⁴

Herein, we present a photochemical molecular rotary motor based on a readily available azoimidazolium salt which operates across a triangular reaction network by taking advantage of the formation of diastereomeric species as a consequence of photoisomerisation. The different thermal stability and photochemical reactivity of the diastereomers allow for net directional motion by combining thermal rotation around a C–N single bond with two photoisomerisation reactions. Additionally, this system can rotate directionally in response to continuous light exposure and can reverse its motion simply by changing the irradiation wavelength.



Figure 1. Graphical representation of the wavelength-steered motion in the investigated rotor.

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Magnetic Levitation Controlled by Light

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Generally known in magnetism are attractive and repulsive forces. The former can be observed in a compass, for example, where the magnetic north pole of the compass needle aligns itself with the earth's magnetic south pole. Another application is in the transportation of magnetic materials, for example by electromagnets in steelworks.

The repulsive forces can also be used to move objects. One example of this are high-speed trains with electromagnets, which move smoothly by means of magnetic levitation (MagLev). In combination with various sensors, precise movement of components in microscopes or robotics can be achieved.^[1]

Mirica *et al.* developed a system with MagLev in which various diamagnetic particles can be examined for their density by placing them in paramagnetic media and converting their levitation height into the specific density.^[2] This setup was combined in the Herges working group with the so-called record player molecules developed there. Those molecules can act as smart contrast agents by initiating a spin crossover in a nickel(II) ion as a result of photoinduced intramolecular coordination (Fig. 1a).^[3] A drop of a dendronized record player molecule could thus be made to levitate and the height could be varied by irradiation with specific wavelengths (Fig. 1b). This system represents the first particle in which the MagLev can be controlled by light.^[4]

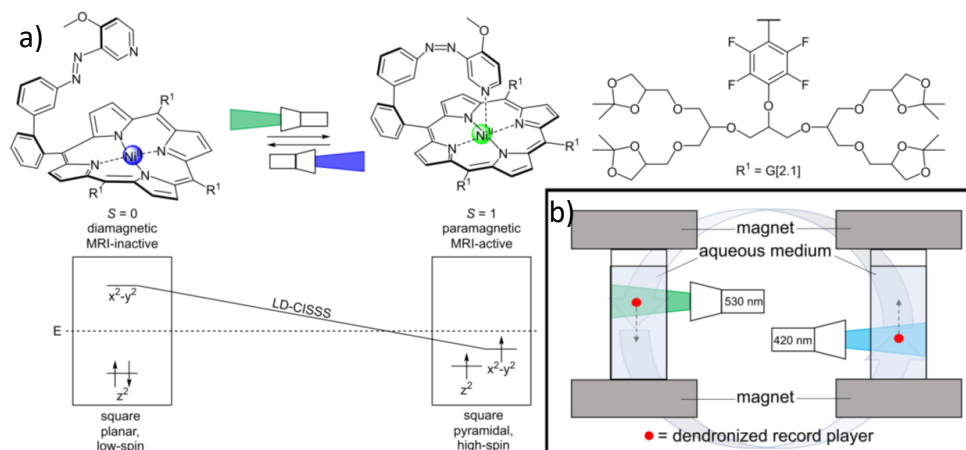


Figure 1. a) Scheme of the switching process of record player molecules. Irradiating with green light initiates a change in the configuration of the azo bond, resulting in an additional coordination at the nickel(II) center and leads to a spin state change (Light Driven-Coordination Induced Spin State Switch)^[3]; b) scheme of the photo switchable magnetic levitation of the dendronized record player molecule.^[4]

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