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GENERAL INFORMATION

INTRODUCTION

The ultimate source of energy on earth is sunlight, but storing solar energy in molecules and soft matter for subsequent use poses a significant challenge. This symposium aims to uncover and explore fundamental concepts that involve utilizing molecules to capture and store light energy. The focus is on any molecular-level interaction with light; relevant topics include the storage of photon energy and the release as heat in molecular solar thermal storage (MOST) systems, as well as transformation photon energy into different types such as chemical or electrical energy.

The symposium will cover, but is not limited to the following themes:

- / Understanding of interactions of light with molecules
- / Molecules involved in light-mediated transformations
- / Photoswitches for energy management
- / Devices utilizing molecules for light-triggered processes

SCIENTIFIC ORGANIZERS

Grace G. D. Han / Brandeis University, Waltham, USA

Hermann A. Wegner / Justus-Liebig-University, Gießen, Germany

WEBSITE

harnessing-light.beilstein-symposia.org

DATES

- | | |
|-----------------------------|-------------------|
| • Scientific program | October 8 to 10 |
| • Traveling days | October 7 and 11 |
| • Welcome dinner | October 7 at 7 pm |

CONFERENCE HOTEL

The conference, lunches and dinners will take place at:

Dom Hotel Limburg Grabenstraße 57 65549 Limburg an der Lahn Germany	T +49 6431 9010 info@domhotellimburg.de www.domhotellimburg.de/en
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ORGANIZATION AND CONTACT

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SCIENTIFIC PROGRAM

Tuesday, October 8

9:00	Welcome and introduction
9:20	Announcement of the winners of the Young Investigator Award
	<i>Session chair: Grace Han</i>
9:30	<u>Solar energy conversion and energy storage materials</u> Kasper Moth-Poulsen / Polytechnic University of Catalunya, Spain
10:10	<u>Converting light energy to mechanical energy with organic molecular crystals</u> Daichi Kitagawa / Osaka Metropolitan University, Japan
10:50	Coffee Break
11:20	<u>Going to the limit - Combining multiple photoswitches</u> Hermann Wegner / Justus-Liebig-University Gießen, Germany
12:00	<u>Tuning the thermal half-life time of Z-isomers of azobenzenes</u> Anne Staubitz / University of Kiel, Germany
12:40	Flash talks for posters #1-7
13:00	Lunch
	<i>Session chair: Rachel Evans</i>
14:15	<u>Molecular design of photoswitches for supramolecular soft matter</u> Bart Jan Ravoo / University of Münster, Germany
14:55	<u>Supramolecular assemblies of photoresponsive molecular amphiphiles</u> Franco King-Chi Leung / The Hong Kong Polytechnic University, China
15:35	Flash talks for posters #8-15
15:55	Coffee Break
16:25	<u>Multiphotochromic molecules incorporating dihydroazulene</u> Mogens Brøndsted Nielsen / University of Copenhagen, Denmark
17:05	<u>Mechanistic investigation of the isomerization of new (and old) photoswitches</u> Stefano Crespi / Uppsala University, Sweden

17:45	Flash talks for posters #16-21
18:05	POSTER SESSION
19:30	End of poster session and dinner

Wednesday, October 9

9:00	Welcome and opening
	<i>Session chair: Bart Jan Ravoo</i>
9:05	<u>A molecular anion pump</u> Ivan Aprahamian / Dartmouth College, USA
9:45	<u>Enzyme-mediated dynamic combinatorial chemistry with cyclodextrins</u> Sophie Beeren / Technical University of Denmark
10:25	<u>Natural product-inspired molecular photoswitch</u> Sunkyu Han / KAIST, Republic of Korea
11:05	Conference photo
11:15	Coffee break
11:45	<u>Molecular solar thermal energy storage (MOST) materials @ Flow chemistry</u> Helen Hölzel / Polytechnic University of Catalonia, Spain
12:25	<u>Insights into MOST systems through theoretical studies</u> Doreen Mollenhauer / Justus-Liebig-University Gießen, Germany
13:05	Lunch
14:45	Excursion Guided tour through the cathedral of Limburg (5 EUR per Person)
19:30	Dinner

Thursday, October 10

9:00	Welcome and introduction
	<i>Session chair: Sunkyū Han</i>
9:05	<u>Optical and spin functions in chromophore assemblies</u> Nobuhiro Yanai / University of Tokyo, Japan
9:45	<u>Coarse-grained modelling for chiral materials design</u> Emma Wolpert / Imperial College London, UK
10:25	<u>Combining the best of organic and inorganic photochemistry with molecular and coulombic dyads</u> Christoph Kerzig / University of Mainz, Germany
11:05	Coffee break
11:35	<u>Designing molecular crystals for solar energy storage and heat release</u> Grace Han / Brandeis University, USA
12:15	<u>Strain engineering of molecular photoswitches for solar thermal energy storage</u> Ravinder Pawar / National Institute of Technology Warangal, India
12:55	Lunch
	<i>Session chair: Hermann Wegner</i>
14:25	<u>Photoswitchable soft self-assembled materials for controlled release and delivery</u> Rachel Evans / University of Cambridge, UK
15:05	<u>On "life-like", light-driven soft actuators</u> Arri Priimägi / Tampere University, Finland
15:45	Coffee break
16:15	<u>Photoresponsive polymers: from photoresists to reversible adhesives</u> Si Wu / University of Science and Technology of China
16:55	<u>From batch to flow: Advancing synthetic organic chemistry through technological innovation</u> Timothy Noël / University of Amsterdam, The Netherlands
17:35	Announcement of the Poster Award winner
19:00	Dinner

ABSTRACTS

Tuesday	Solar energy conversion and energy storage materials
9:30	Kasper Moth-Poulsen
	Polytechnic University of Catalunya, Barcelona, Spain

Since the beginning of civilization, humanity has built houses to sustain comfortable living conditions throughout the seasons. In our modern society, about 50% of the total energy consumption is used for heating and cooling. Growing demands for thermal management in many different sectors, from electronics to housing, inevitably mean increased energy consumption. The primary source of heat is coming from the combustion of fossil, bio or waste-based feedstocks, all contributing to carbon emissions.

In this lecture I will present how we are working on developing molecular materials that capture, store, and release both solar and ambient heat without creating any emissions. These molecular solar thermal systems (MOST) are based on molecular photoswitches that absorb light and convert it into stored chemical energy, that can be released on demand.[1-6] The MOST energy system operates through different principles than traditional solar thermal and can be introduced into compact energy capture and release devices. Recently, the first example of integration of the energy storage system with photovoltaics, and in electric power generation devices was published.[7-8] Additionally, I will introduce materials concepts for photon upconversion (TTA-UC) and associated accelerated discovery devices.

References:

- [1] Z. Wang *et al.* *Energy Environ. Sci.* **2019**, *12*, 187-193, doi: 10.1039/C8EE01011K (cover)
- [2] Mads Mansø *et al.* *Nat. Commun.* **2018**, *9*, 1945, doi: 10.1038/s41467-018-04230-8.
- [3] Ambra Dreos *et al.* *Energy Environ. Sci.* **2017**, *10*, 728-734, doi: 10.1039/C6EE01952H. (cover)
- [4] Anne Ugleholdt Petersen *et al.* *Adv. Sci.* **2019**, *12*, 1900367, doi: 10.1002/advs.201900367.
- [5] Zhao-Yang Zhang *et al.* *J. Am. Chem. Soc.* **2020**, *142*, 12256–12264, doi: 10.1021/jacs.0c03748.
- [6] Zhihang Wang *et al.* *Joule* **2021**, *5*, 3116-3136, doi: 10.1016/j.joule.2021.11.0012021.
- [7] Z. Wang *et al.* *Joule* **2024**, doi: 10.1016/j.joule.2024.06.012.
- [8] Zhihang Wang *et al.* *Cell Rep. Phys. Sci.* **2022**, *3*, 100789, doi: 10.1016/j.xcrp.2022.100789

Tuesday

**Converting light energy to mechanical energy
with organic molecular crystals**

10:10

Daichi Kitagawa

Osaka Metropolitan University, Japan

Organic molecular crystals that respond to external stimuli have drawn tremendous attention as next-generation functional materials because they exhibit interesting phenomenon such as superelasticity, self-healing, fluorescence color change, gas adsorption/desorption, and so on. Among them, we have so far conducted the research on the photomechanical behavior of crystals, in which the shape of the crystal changes in response to light irradiation. Photomechanical crystals can convert light energy to mechanical energy via photochemical reactions and have potential applications in artificial muscles and microrobots. In addition, they have superior actuator performances such as fast response speeds, high energy densities and reasonable photon-to-work conversion efficiencies when compared to other photomechanical materials like liquid-crystalline polymers, amorphous or semicrystalline polymers, and gels. In this paper, we review the progress in the field of photomechanical crystals over the past 20 years, including our own research findings.[1] Moreover, we introduce our recent studies on the analysis of photochemical reaction kinetics in the crystalline state that is essential to understand the relationship between photochemical reaction kinetics and the photomechanical response dynamics.[2]

References:

- [1] a) D. Kitagawa *et al.* *Angew. Chem. Int. Ed.* **2013**, *52*, 9320-9322, doi: 10.1002/anie.201304670; b) D. Kitagawa *et al.* *Am. Chem. Soc.* **2018**, *140*, 4208-4212, doi: 10.1021/jacs.7b13605; c) F. Tong *et al.* *Angew. Chem. Int. Ed.* **2018**, *57*, 7080-7084, doi: 10.1002/anie.201802423; d) X. Dong *et al.* *Chem. Mater.* **2019**, *31*, 1016-1022, doi: 10.1021/acs.chemmater.8b04568; e) W. Xu *et al.* *Nat. Mater.* **2023**, *22*, 1152-1159, doi: 10.1038/s41563-023-01610-4; f) F. Tong *et al.* *Angew. Chem. Int. Ed.* **2021**, *60*, 2414-2423, doi: 10.1002/anie.202012417.
- [2] a) K. Morimoto *et al.* *Angew. Chem. Int. Ed.* **2022**, *61*, e202114089, doi: 10.1002/anie.202114089; b) K. Morimoto *et al.* *Angew. Chem. Int. Ed.* **2022**, *61*, e202212290, doi: 10.1002/anie.202212290; c) S. Kataoka *et al.* *Chem. Sci.* **2024**, *15*, 13421-13428, doi: 10.1039/D4SC03060E.

Tuesday

Going to the limit – Combining multiple photoswitches

11:20

Hermann A. Wegner

Justus-Liebig-University Gießen, Germany

Light offers the cleanest and most selective way to introduce energy into matter. Especially, if a specific reaction or function is triggered, such as in a photoswitch. Photoswitches offer limitless possibilities in medicinal, biological or materials science. An intriguing aspect is the potential of molecular photoswitches for storage applications. In this context the density of information or energy is crucial. Generally, each molecular switch occupies its own specific structural space. But what if multiple switches could be integrated to share the same space? Over the past few years, we have investigated this concept by combining various photoswitches with azobenzenes. We have pushed this idea to the point where two switches can operate using the same molecular structures. Examples of such switches include inter alia other azobenzenes,[1,2,3] norbornadienes,[4] and spiropyrans.[5] This integration of multiple switches, or "mostophores," presents an effective strategy for increasing the energy density in molecular solar thermal (MOST) candidates. Opportunities and challenges will be presented.

References:

- [1] C. Slavov *et al.* *Phys. Chem. Chem. Phys.*, **2016**, *18*, 14795-14804, doi: 10.1039/C6CP00603E.
- [2] C. Yang *et al.* *Chem. Sci.*, **2018**, *9*, 8665-8672, doi: 10.1039/C8SC03379J.
- [3] A. Kunz *et al.* *Chem. Eur. J.* **2022**, e202200972, doi: 10.1002/chem.202200972.
- [4] A. Kunz, *et al.* *ChemSystemsChem*, **2020**, *2*, e2000035, doi: 10.1002/syst.202000035.
- [5] T. Saßmannshausen *et al.* *Angew. Chem. Int. Ed.* **2024**, *63*, e202314112, doi: 10.1002/anie.202314112.

Tuesday	Tuning the thermal half-life time of Z-isomers of azobenzenes
12:00	Anne Staubitz
	University of Kiel, Germany

Azobenzenes can switch between a (usually) more stable *E*-isomer and a less stable *Z*-isomer using different wavelengths. However, there is also a thermal relaxation pathway from the *Z*- to the *E*-isomer, which limits the use of this switch as an information storage material or energy storage material. This presentation will discuss the influence of substituents and the incorporation of the azobenzene in a macrocycle on the thermal half-life time.[1, 2] The current record is a thermal half-life time of ca. 120 years at room temperature.[3]

References:

- [1] N. Eleya *et al.* *J. Mater. Chem. C* **2021**, *9*, 82-87, doi: 10.1039/d0tc05211f.
 [2] S. Ghosh *et al.* *J. Org. Chem.* **2023**, *88*, 3372-3377, doi: 10.1021/acs.joc.2c00549.
 [3] S. Schultze *et al.* *Adv. Funct. Mater.* **2024**, *34*, 2313268, doi: 10.1002/adfm.202313268.

Tuesday	Molecular design of photoswitches for supramolecular soft matter
14:15	Bart Jan Ravoo
	University of Münster, Germany

Self-assembly is emerging as a superior method to prepare responsive and adaptive nanomaterials. The structure and function of these materials is entirely determined by the dynamic and weak interactions of the constituent molecular “building blocks” of the material. Since the inherent interactions are weak, these versatile materials readily respond to even small changes and stimuli in their environment.

This lecture will highlight our recent work on self-assembled supramolecular nanomaterials that respond and adapt to light. In all these nanomaterials, molecular photoswitches are key components. The improved molecular design of photoswitches enables the bottom-up self-assembly of tailor-made functional materials and interfaces that can be manipulated with light. Amongst others, light responsive surfactants, liquid crystals, adhesives and solids will be discussed. Also, the optical manipulation of cell shape with light will be addressed.

References:

- Mukherjee *et al.* *Angew. Chem. Int. Ed.* **2023**, *25*, e202304437, doi: 10.1002/anie.202304437.

Tuesday	Supramolecular assemblies of photoresponsive molecular amphiphiles
14:55	Franco King-Chi Leung
	The Hong Kong Polytechnic University, China

Recent advancements in supramolecular chemistry and soft functional materials design have enabled various supramolecular assembling systems responsive to external stimuli, e.g., light, heat, pH, small organic molecules, and ions. Among the various external stimulations, light provides as a non-invasive method with high-spatial and high-temporal precision in controls of supramolecular assembling structures in both organic and aqueous media. Implementations of photoresponsive molecular functionalities into molecular amphiphilic motifs, i.e., photoresponsive molecular amphiphile, have constructed a series of synthetic photoresponsive supramolecular systems at air-water interface and in aqueous media, enabling controlled interfacial properties, reversible nanoscale assembly, and artificial muscle functions. Some of these photoresponsive molecular amphiphiles are capable to assemble across multiple length-scale, fabricating photoresponsive soft materials at macroscopic length-scale. However, the biocompatibility remains unsolved in the reported bio-damaging UV-light activated systems. We discuss our recent works on the biocompatible supramolecular actuator of photoresponsive DASA amphiphiles[1] and other visible-light controlled supramolecular soft materials.[2]

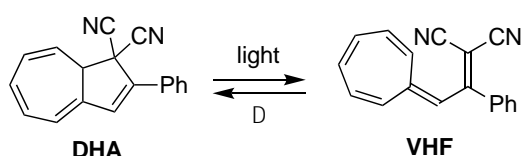
References:

- [1] K.-L. Hung *et al.* *Beilstein J. Org. Chem.* **2024**, *20*, 1590–1603, doi: 10.3762/bjoc.20.142.
 [2] (a) L.-H. Cheung *et al.* *ACS Appl. Mater. Interfaces* **2024**, *16*, 4056–4070, doi: 10.1021/acsmi.3c16795; (b) J. C.-K. Yau *et al.* *J. Colloid Interface Sci.* **2024**, *662*, 391–403, doi: 10.1016/j.jcis.2024.02.075; (c) L.-H. Cheung *et al.* *J. Colloid Interface Sci.* **2022**, *628*, 984–993, doi: 10.1016/j.jcis.2022.08.034.

Tuesday	Multiphotochromic molecules incorporating dihydroazulene
16:25	Mogens Brøndsted Nielsen
	University of Copenhagen, Denmark

Multiphotochromic molecules consist of two or more molecular photoswitches connected covalently together and are promising candidates for molecular solar thermal (MOST) energy storage applications or for advanced optical data storage.[1] The usually extended conjugation of the systems usually allows for stronger absorptions in the visible region and hence a better

match with the solar spectrum. Moreover, higher energy densities of MOST systems may be obtained with such systems in comparison to the sum of energy densities of the individual photochromic units as some structural parts are shared between the units. The photochromic units may interact and control each other, allowing for stepwise photoisomerizations. In this talk, I will focus on our work on multiphotochromic molecules incorporating the dihydroazulene/vinylheptafulvene (DHA/VHF) photo-/thermoswitch couple.[2] DHA undergoes a light-induced ring-opening reaction to form a vinylheptafulvene that thermally in time will return to DHA. Systems with two or more DHA units[3] will be covered as well as combinations with azobenzene,[4] norbornadiene,[5] or spiropyran photoswitches.[6] Tuning of switching properties by introducing DHA units within macrocycles will also be covered.[7]



References:

- [1] a) A. H. Heindel, H. A. Wegner, "Multinary Photoswitches" in *Molecular Photoswitches: Chemistry, Properties, and Applications* (Ed. Z. L. Pianowski), Wiley-VCH, **2022**; b) R. J. Salthouse *et al. J. Mater. Chem. A* **2024**, *12*, 3180-3208, doi: 10.1039/D3TA05972C.
- [2] a) S. L. Broman *et al. Phys. Chem. Chem. Phys.* **2014**, *16*, 21172-21182, doi: 10.1039/C4CP02442G; b) M. B. Nielsen *et al. Russ. Chem. Rev.* **2020**, *89*, 573-586, doi: 10.1070/RCR4944.
- [3] a) A. U. Petersen *et al., Chem. Eur. J.* **2015**, *21*, 3968-3977, doi: 10.1002/chem.201405457; b) A. U. Petersen *et al. Chem. Eur. J.* **2020**, *26*, 13419-13428, doi: 10.1002/chem.202000530.
- [4] A. Mengots *et al., Chem. Eur. J.* **2021**, *27*, 12437-12446, doi: 10.1002/chem.202101533.
- [5] M. D. Kilde *et al. Org. Biomol. Chem.* **2019**, *17*, 7735-7746, doi: 10.1039/C9OB01545K.
- [6] M. Dowds *et al. ChemPhotoChem* **2022**, *6*, e202200152, doi: 10.1002/cptc.202200152.
- [7] a) A. Vlasceanu *et al. Chem. Eur. J.* **2016**, *22*, 10796-10800, doi: 10.1002/chem.201602512; b) A. Vlasceanu *et al. J. Org. Chem.* **2017**, *82*, 10398-10407, doi: 10.1021/acs.joc.7b01760; c) M. Cacciarini *et al. Chem. Commun.* **2017**, *53*, 5874-5877, doi: 10.1039/C7CC01050H; d) A. Vlasceanu *et al. Angew. Chem. Int. Ed.* **2018**, *57*, 6069-6072, doi: 10.1002/anie.201712942.

Tuesday

Mechanistic investigation of the isomerization of new (and old) photoswitches

17:05
Stefano Crespi

Uppsala University, Sweden

Photochemically driven molecular switches and unidirectional molecular motors represent a fascinating fundamental research topic.[1,2] These small chromophores can drive the dynamics of molecular systems and devices at the nanoscale, a peculiar feature that has found applications in smart materials and biomedical sciences. However, synthesizing molecules tuned for a specific task requires a deep understanding of their motion.

This talk will focus on selected examples of applying the toolboxes offered by organic synthesis, spectroscopy, computational chemistry and physical organic chemistry to predict, construct and investigate photochemically driven switches and motors (Fig. 1).[3-7] This approach allows the understanding of the behavior of new structures and the discovery of the mechanisms underlying their movement at the molecular scale.

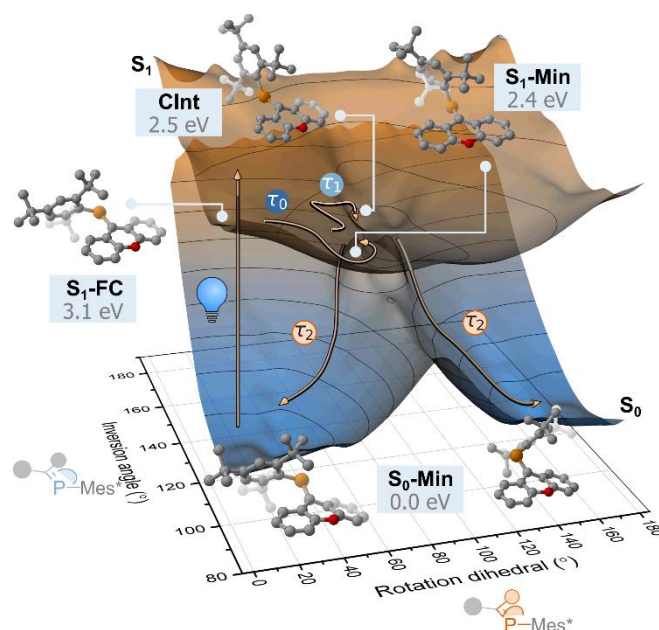


Figure 1: Potential energy surface associated with the isomerization about the central C=P bond of a novel molecular switch obtained at the MRSF-TDDFT/6-31G* level.

References:

- [1] S. Crespi *et al.* *Nat. Rev. Chem.* **2019**, *3*, 133, doi: 10.1038/s41570-019-0074-6.
- [2] D. R. S. Pooler *et al.* *Chem. Sci.* **2021**, *12*, 14964, doi: 10.1039/D1SC04781G.
- [3] S. Crespi *et al.* *Angew. Chem. Int. Ed.* **2021**, *60*, 25290, doi: 10.1002/anie.202111748.
- [4] L. Pfeifer *et al.* *Nat. Commun.* **2022**, *13*, 2124, doi: 10.1038/s41467-022-29820-5.
- [5] M. Kathan *et al.* *Nat. Nanotech.* **2022**, *17*, 159, doi: 10.1038/s41565-021-01021-z.
- [6] K. Kuntze *et al.* *Chem. Sci.*, **2023**, *14*, 8458, doi: 10.1039/D3SC03090C.
- [7] A. Volker *et al.* *Beilstein J. Org. Chem.* **2024**, *20*, 1684, doi: 10.3762/bjoc.20.150.

Wednesday

A molecular anion pump

9:05
Ivan Aprahamian

Dartmouth College, Hanover, USA

Pumping ions against a concentration gradient is a cornerstone of numerous biological processes.[1] Using artificial receptors to replicate such ion pumping is a daunting challenge because of the strict requirements for high binding affinities, and precise on-demand ion capture and release.[2] In this talk I will discuss the development of a trimeric hydrazone-based[3] receptor (Figure 1) that actively transports chloride anions against a concentration gradient, thus converting light energy into work, and subsequently functioning as a molecular chloride pump.[4,5]

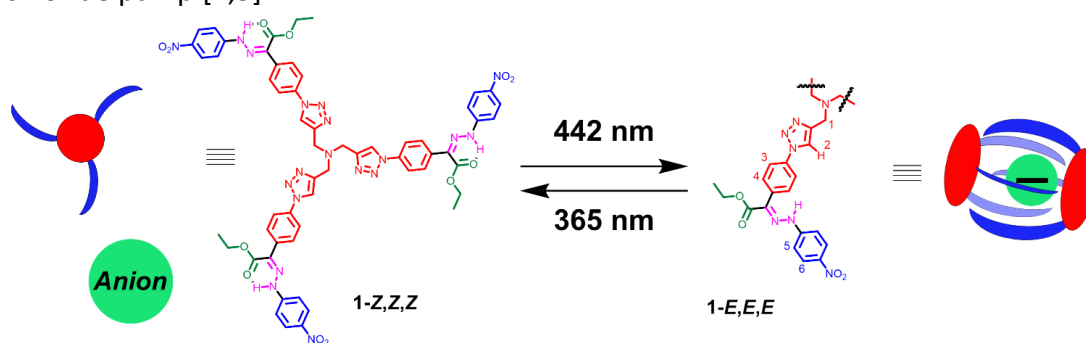


Figure 1: The hydrazone receptor in its Z form cannot bind to anions. Upon switching to the E configuration using visible light a six-order of magnitude increase in binding to chloride is observed, facilitated among other things by the formation of a 2:1 complex.

References:

- [1] D. C. Gadsby, *Nat. Rev. Mol. Cell. Biol.*, **2009**, 10, 344–352, doi: 10.1038/nrm2668.
- [2] J. T. Davis *et al.* *Chem. Soc. Rev.*, **2020**, 49, 6056–6086, doi: 10.1039/C9CS00662A.
- [3] B. Shao *et al.* *Chem*, **2020**, 6, 2162–2173, doi: 10.1016/j.chempr.2020.08.007.
- [4] I. Aprahamian, *ACS Cent. Sci.* **2020**, 6, 347–358, doi: 10.1021/acscentsci.0c00064.
- [5] B. Shao *et al.* *Science*, **2024**, 385, 544–549, doi: 10.1126/science.adp3506.

Wednesday

Enzyme-mediated dynamic combinatorial chemistry with cyclodextrins

9:45
Sophie Beeren

Technical University of Denmark, Kongens Lyngby, Denmark

Biomolecular templates define the outcomes of enzymatic reactions in some of the most fundamental of biological processes, such as DNA replication, transcription and translation. In synthetic chemistry, molecular templates have enabled the synthesis of highly complex molecular architectures and interlocked structures. With *Enzyme-Mediated Dynamic Combinatorial Chemistry*, we explore the possibility of using synthetic templates to direct enzymatic reactions and obtain alternative products to those generated in nature.

α -, β - and γ -cyclodextrin are industrially important macrocyclic hosts formed from 6, 7, and 8 α -1,4-linked glucopyranose units. While cyclodextrins are usually considered as stable, static molecules, we generate dynamic mixtures of interconverting cyclodextrins by the action of *cyclodextrin glucanotransferase* (CGTase). As the system is dynamic, the product distribution can be manipulated via supramolecular interactions with template molecules.[1] We use templates to direct the selective synthesis of 'natural' cyclodextrins as well as modified cyclodextrins, and employ photoswitches as templates, in order to control the system using light.[2]

While α -, β - and γ -cyclodextrin (CD) are well-known macrocyclic hosts with wide-ranging applications, large-ring cyclodextrins, formed from more than 8 glucose units, have received limited attention due to synthetic inaccessibility. We show how d-CD (formed from 9 glucose units) and e-CD (formed from 10 glucose units) can be synthesized in unprecedented yields by employing specifically designed templates to direct the dynamic enzymatic synthesis of cyclodextrins towards these larger macrocycle.[3] We can now convert α -CD to d-CD in 40% yield via a single reaction step and on a multi-gram scale.[4] Investigations are ongoing to explore the molecular recognition capabilities of this newly accessible macrocyclic host.

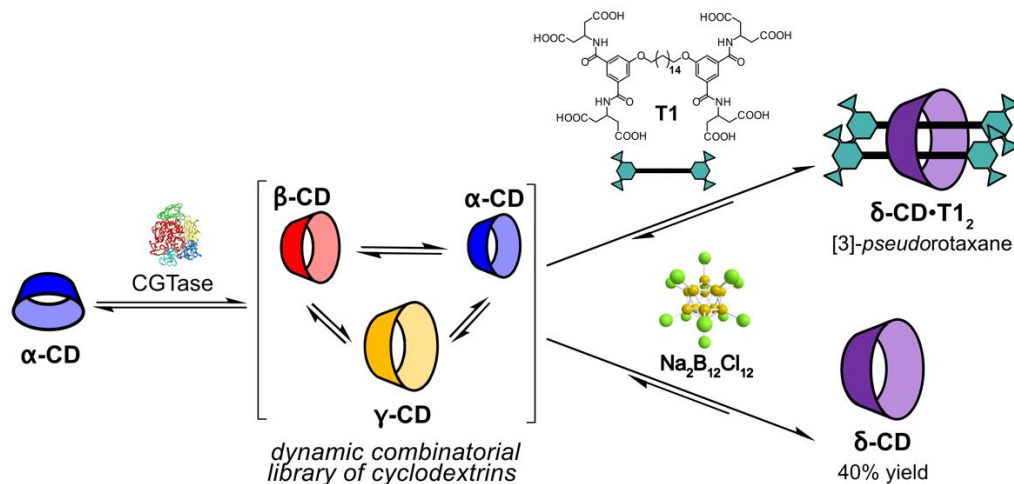


Figure 1. Template-directed enzymatic synthesis of d-cyclodextrin.

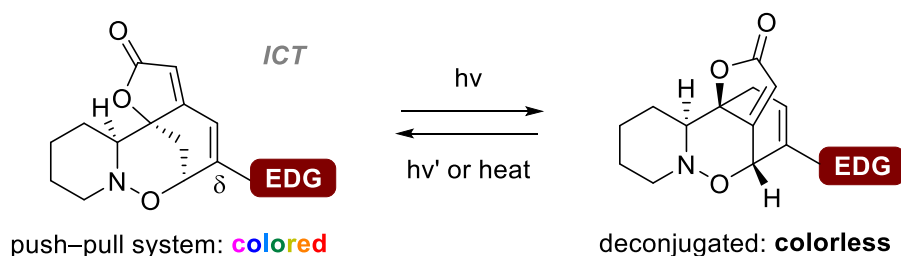
References:

- [1] D. Larsen *et al.* *Chem. Sci.*, **2019**, *10*, 9981–9987, doi: 10.1039/C9SC03983J.
- [2] J. Sørensen *et al.* *Chem. Sci.*, **2023**, *14*, 7725–7732, doi: 10.1039/D3SC01997G.
- [3] A. Erichsen *et al.* *J. Am. Chem. Soc.*, **2023**, *145*, 4882–4891, doi: 10.1021/jacs.3c00341.
- [4] K. Hansen, A. Erichsen, D. Larsen, S. R. Beeren, ‘Method for the production of large-ring cyclodextrins’ **2024**, WO/2024/042228.

Wednesday	Natural product-inspired molecular photoswitch
10:25	Sunkyu Han
	KAIST, Daejeon, Republic of Korea

Natural product synthesis has long been pivotal in drug discovery, providing key principles and compounds that have driven the development of new therapeutics. In this study, we show that the synthetic exploration of natural products can also extend beyond the realm of pharmaceuticals. We reveal how this approach can lead to the invention of innovative molecular photoswitches.

By leveraging the higher triplet energy of contra-thermodynamic securinine B relative to the more thermodynamically stable secu’amamine D, we achieved a highly efficient photochemical transformation of secu’amamine D to securinine B. Conversely, securinine B was converted back to secu’amamine D under conditions that favor thermodynamic equilibrium. Building on these novel reactivities, we developed a new photoswitching platform by integrating a push-pull system into the securinega framework. This novel photoswitching system was applied into the development of unprecedented photochromic materials and photoresponsive chiral dopants for liquid crystals.


References:

- [1] S. Park, G. Kang, W. Kim, S. Jeon, M. K. Chung, H.S. Lee, D. K. Yoon, S. Han, in revision.
- [2] G. Kang *et al.* *Acc. Chem. Res.* **2023**, *56*, 140, doi: 10.1021/acs.accounts.2c00719.
- [3] S. Park *et al.* *Nat. Commun.* **2022**, *13*, 5149, doi: 10.1038/s41467-022-32902-z.

Wednesday

Molecular solar thermal energy storage (MOST) materials @ Flow chemistry

11:45

Helen Hölzel

Polytechnic University of Catalonia, Barcelona, Spain

Molecular solar thermal energy storage systems (MOST), also known as solar thermal fuels (STF) attract increasing attention due to their possible and promising use regarding solar energy harvesting and more significantly storage.[1] Solar irradiation is used to excite the MOST material which then undergoes a chemical reaction to result in an energy-rich metastable isomer that can store the energy and release it on demand via triggered back-reaction, to restore the parent molecular state. Examples of their actual implementation into proof-of-principle devices have been shown to demonstrate their potential.[2] On the other hand, a novel technique, flow chemistry, takes on greater significance, especially due to several advantages over usual batch chemistry. Herein, we present materials for MOST and the use of flow techniques, both, individually and in synergy (Figure 1b), highlighting e.g. synthesis and optimization, and the investigation of MOST materials using standard analysis and emerging flow techniques.[3,4] Besides other, examples based on the norbornadiene (NBD)/quadricyclane (QC) photoisomerization pair will be on display.

References:

- [1] Z. Wang *et al.* *Joule* **2021**, *5*, 3316-3136, doi: 10.1016/j.joule.2021.11.001.
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Wednesday**Insights into MOST systems through theoretical studies****12:25****Doreen Mollenhauer**

Justus-Liebig-University Gießen, Germany

In the development of MOST-based storage technologies, it is important to understand the underlying MOST pairs in detail in order to optimise the storage energy, control the energy barriers and tune the catalytic energy release. In this context, quantum chemical calculations can support the design of novel MOST systems, as well as the investigation of surface-driven catalytic processes and the influence of intra- and intermolecular non-covalent interactions on MOST properties. Our results from theoretical studies of single molecules, interacting molecules and surface processes provide in-depth structural, energetic and property insights into different MOST systems and also aid in the design of novel MOST systems.[1]

Reference:

[1] E. Franz *et al.* *J. Phys. Chem. Lett.* **2023**, *14*, 1470, doi: 10.1021/acs.jpcllett.2c03732.

Thursday**Optical and spin functions in chromophore assemblies****9:05****Nobuhiro Yanai**

University of Tokyo, Japan

Excited triplets of organic molecules have the interesting features of long excitation lifetime and spin polarization. Among various functions of excited triplets, our recent works on the development of chromophore assemblies exhibiting photon upconversion and singlet fission will be presented. Triplet-triplet annihilation based photon upconversion (TTA-UC) from visible light to UV light is useful for various photocatalysts including artificial photosynthesis, but its low efficiency (<10%) has been a problem for several years. We have developed a chromophore pair that exhibits a high TTA-UC efficiency of over 20%, which is two times higher than the previous record for Vis-to-UV TTA-UC. The Ir coumarin complex shows strong absorption in the visible range and relatively weak absorption in the UV range and does not quench the upconverted UV emission. By combining the Ir coumarin complex with TIPS-naphthalene, we have achieved a high TTA-UC efficiency of over 20% and a very low threshold excitation intensity below solar irradiance. Focusing on the excellent absorption properties of coumarin derivatives, we have also succeeded in achieving a high TTA-UC efficiency of more than 20% without using heavy metals by employing a heavy metal-free sensitizer modified with a carbonyl group on coumarin.

We are also interested in the spin degree of freedom of singlet fission in the context of quantum information science (QIS). We developed chromophore assemblies and dimers exhibiting singlet fission, and successfully observed quantum coherence of quintet triplet dimer state at room temperature for the first time. We found that the suppressed chromophore dynamics is crucial for achieving both of quintet formation and quantum coherence.

Thursday	Coarse-grained modelling for chiral materials design
9:45	Emma Wolpert
	Imperial College London, UK

The optoelectronic properties of pi-conjugated molecules are highly anisotropic and as such, the orientation of the molecules can severely impact their functionality. Recent studies [1,2,3] have shown that both inorganics and organic materials can be used as a templating layer to control the supramolecular organisation of chiral and planar aromatic systems. Understanding how different surfaces and molecules interact remains a non-trivial task due to the large computational expense required for accurate calculations.

Coarse-grained models are widely used to reduce the computational cost of simulating materials phase behaviour whilst retaining the main chemical and physical degrees of freedom. But beyond reducing computational cost, coarse-grained models can also be used to develop design rules by highlighting the degrees of freedom which are responsible for materials phase behaviour. Here we show how coarse-grained models can be used for molecular materials design by relating molecules to rigid shapes with directional interactions and simulating their assembly in the solid state and on surfaces. Our results show we can recreate the structure of materials seen in the literature, highlighting the potential for this model to predict the assembly of new molecules, inform design rules, and motivate targeted design.

References:

- [1] D. K. Kim *et al. Mater. Horiz.* **2020**, *7*, 289-298, doi: 10.1039/C9MH00355J.
- [2] J. Wade *et al. Nat. Chem.* **2022**, *14*, 1383-1389, doi: 10.1038/s41557-022-01044-6.
- [3] L. Rochford *et al. Adv. Mater. Interfaces* **2015**, *2*, 1400540, doi: 10.1002/admi.201400540.

Thursday

Combining the best of organic and inorganic photochemistry with molecular and coulombic dyads

10:25

Christoph Kerzig

University of Mainz, Germany

Dyads or bichromophores can be designed such that unique properties for photochemical energy and electron transfer reactions result. These properties are based on the interplay of an inorganic chromophore, enabling quantitative intersystem crossing as well as visible light absorption, and a covalently linked organic moiety with a long-lived triplet state. We synthesized ruthenium complex-based molecular dyads decorated with a covalently attached pyrene chromophore and used them for efficient photooxygenations in water, which is a challenging solvent for such reactions.[1] The long-lived pyrene triplets in these dyads are relatively redox-inert compared to the MLCT triplets of the parent metal complexes. Hence, these dyads provide an efficient access to acceptor triplet states that are otherwise very tricky to obtain, which allowed us to establish a triplet quenching pathway control approach with molecular dyads.[2] Guided by our recent study on coulomb effects on the energy transfer kinetics,[3] we have developed a novel strategy for obtaining the advantages of molecular dyads without the time- and resource-consuming synthesis of these tailored photocatalysts. Simply by mixing a cationic ruthenium complex with an anionic pyrene derivative in water a salt bichromophore is produced owing to electrostatic interactions. We exploited this so-called Coulombic dyad for several photoreactions in the context of light-to-energy conversion with outstanding reaction quantum yields and turnover numbers.[4] In the last part of my talk, our recent findings on triplet-sensitized MOST systems will be presented.

References:

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- [2] M.-S. Bertrams *et al.* *Chem. Sci.* **2023**, 14, 8583–8591, doi: 10.1039/D3SC01725G.
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Thursday**Designing molecular crystals for solar energy storage and heat release****11:35****Grace Han**

Brandeis University, Waltham, USA

In our recent studies, we have showcased various topochemical reactions, including [2+2] and [4+4] photocycloadditions, which effectively store solar photon energy in the crystalline state of molecules. The triggered cycloreversion releases the stored energy as heat, and some systems exhibit a unique self-activated heat release and propagation. The presentation will introduce molecular design principles that facilitate reversible topochemical cycloadditions in solids. Furthermore, mechanistic and kinetic analysis of the self-catalyzed cycloreversion process will be illustrated. Lastly, the energy storage densities will be compared among the different molecular systems and attributed to their chemical and physical transformations.

Thursday**Strain engineering of molecular photoswitches for solar thermal energy storage****12:15****Ravinder Pawar**

National Institute of Technology Warangal, India

Energy is an inevitable necessity whose rate of consumption is continuously increasing across the world.[1] Excessive consumption of fossil fuels present significant environmental challenges and poses a risk of depleting natural reserves thus, necessitates transition towards a powerful and sustainable energy source.[1,2] Albeit the Sun is a renewable and potent energy resource that powers the earth, the lack of technology for efficient light-harvesting remains a barrier to its direct utilization.[3] Designing photoswitches for molecular solar thermal (MOST) systems is currently the heart of several investigations, offering the potential to harness and store solar energy for extended periods.[4,5] Understanding the interplay between molecular structure, strain, and properties is crucial to simplify the approach towards achieving our goal of photoswitch designing for practical MOST systems. Herein, we made an attempt to elucidate these relationships, providing guidance for rational designing of the core molecular skeletons to bestow desirable features in a single photoswitching couple. By applying the insights gained from these correlations, we explore experimentally accessible photoswitching systems, paving the way for future experimental investigations and applications in MOST technologies.

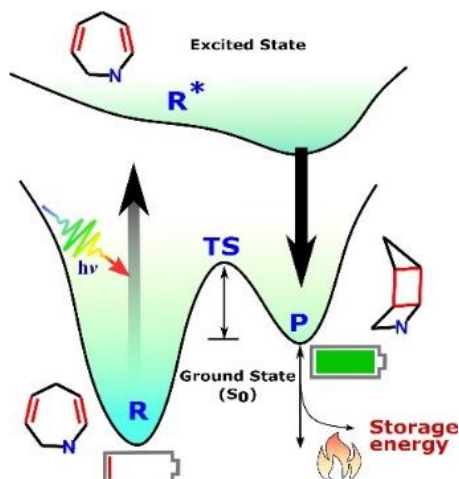


Figure 1: Photoswitching cycle for MOST application.

References:

- [1] N. S. Lewis *et al.* *Proc. Natl. Acad. Sci. U.S.A.* **2006**, *103*, 15729–15735, doi: 10.1073/pnas.0603395103.
- [2] M. Grätzel, *Nature* **2000**, *403*, 363, doi: 10.1038/35000273.
- [3] J. Su *et al.* *ACS Energy Lett.* **2016**, *1*, 121–135, doi: 10.1021/acsenergylett.6b00059.
- [4] Z. Wang *et al.* *Chem. Soc. Rev.* **2022**, *51*, 7313–7326, doi: 10.1039/D1CS00890K.
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Thursday	Photoswitchable soft self-assembled materials for controlled release and delivery
14:25	Rachel Evans
	University of Cambridge, UK

Light-responsive systems that deliver a function are ubiquitous in nature, for example the photoisomerisation of retinal in the eye that leads to vision, or the phototropic growth of sunflowers. As such, there is considerable interest in developing synthetic materials that can mimic such behaviour to design smart technologies that are powered by light. In particular, the integration of photoactive molecules into dynamic, self-assembled soft materials presents the opportunity to translate molecular level sensitivity across hierarchical length scales.

In this talk, recent highlights from our group to design new photoresponsive colloidal materials operating over different length scales for controlled release and delivery will be described. It will be shown that the incorporation of photoswitches such as azobenzene (Azo)[1] or arylazopyrazole (AAP)[2] into a surfactant structure results in the unique combination of surface activity, self-assembly and *trans-cis* photoisomerisation in a single molecule. These photosurfactants (PS) demonstrate the combined ability to change their shape upon irradiation with light and to self-organise into polymolecular assemblies such as

lyotropic liquid crystals (LLCs).[3] We first demonstrate that AzoPS can be combined with lipids to produce light-responsive cubic LLC dispersions, in which the AzoPS allows external control over the LLC nanostructure and subsequent on-demand release of entrapped guest molecules.[4] We then show that AzoPS-functionalised silica nanoparticles can be used to form particle-stabilised emulsion (micrometer) droplets, that can be deformed and reformed through the remote application of light.[5] Finally, we demonstrate that light-driven phase switching in AAP LLCs can be used to control the diffusion of gases across membranes.[6]

References:

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 [2] G. Tyagi *et al.* *JACS Au*, **2022**, *2*, 2670–2677, doi: 10.1021/jacsau.2c00453.
 [3] J. E. Houston *et al.* *J. Mater. Chem. C*, **2019**, *7*, 10945–10952, doi: 10.1039/C9TC04079J.
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 [6] B. E. Jones *et al.* *J. Am. Chem. Soc.* **2024**, *146*, 12315–12319, doi: 10.1021/jacs.4c02709.

Thursday	On "life-like", light-driven soft actuators
15:05	Arri Priimägi
	Tampere University, Finland

Biological systems, viewed within the materials science perspective, are excessively complex. They are adaptive, multifunctional and -responsive, dissipative, self-regulating, and capable of evolving and learning from their past experiences. Hence, biological systems have provided a great source of inspiration for scientists aiming to design functional and “intelligent” materials. Liquid crystal network (LCN) and hydrogel-based soft actuators provide a rich platform for simplistically mimicking some of the properties of natural systems, as demonstrated by examples of systems that are deemed feedback-driven, autonomous, adaptive, self-regulating, or capable of “learning”. Such materials can be deemed “life-like” (or life-inspired?) in a simplified sense. Yet again, they fall way short on their natural counterparts in terms of dynamism, complexity, capability to respond to environmental cues, and to evolve based on past experiences. The aim of this talk is twofold, both of which are approached using our own work on light-responsive LCN actuators as an example. On one hand, it will be shown how even very simple supramolecular concepts can enhance the complexity and (multi)functionality of the systems. On the other hand, I try to reflect upon the question, or provoke discussion, on whether the terminology stemming from living systems is justified or useful in the context of fully synthetic soft actuators.

Thursday

Photoresponsive polymers: from photoresists to reversible adhesives

16:15

Si Wu

University of Science and Technology of China, Hefei, China

In this talk, I would like to introduce the synthesis of photoresponsive polymers and control of their functions with light.[1-6] First, I will present that light can induce reversible solid-to-liquid transitions of azopolymers. The azobenzene groups in the polymers exhibit reversible cis–trans photoisomerization. Trans azopolymers are solids, whereas cis azopolymers are liquids. These azopolymers can be applied to healable materials, reprocessable materials and photoresists for nanoimprint lithography. I will show a few examples about nanopatterns fabricated using azopolymers via nanoimprint lithography. Second, I will introduce photoresponsive metallopolymers based on Ru-N, Ru-Se and Ru-S bonds. These bonds are stable in the dark and can reversibly dissociate under light irradiation. These coordination bonds are promising building blocks for dynamic materials, which are applicable to different operating environments. We prepared photoresponsive polymer gels using Ru complexes as crosslinks. Polymer gels underwent photoinduced reversible sol-gel transitions, which can be used for reversible adhesives. Soft robotics are prepared by gluing responsive hydrogel units with reversible adhesives.

References:

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Thursday

From batch to flow: Advancing synthetic organic chemistry through technological innovation

16:55

Timothy Noël

University of Amsterdam, The Netherlands

The world of synthetic organic chemistry has made significant strides in discovering new medicines, materials, and fine chemicals. However, there is a major aspect that has been overlooked for years - the reactor itself. In this talk, we will explore the potential of flow chemistry to advance synthetic organic chemistry through technological innovation.

By harnessing the power of flow chemistry, chemists can unlock unique reactivity and selectivity, enabling them to push the boundaries of what is possible.[1] Not only does flow chemistry make new synthetic routes achievable, it can fast-track them from the lab to large scale production.[2]

At our research group, we are committed to advancing the field by developing automated and flow-based reaction technologies that reduce manual labor, increase reproducibility, and accelerate reaction discovery. Our focus on flow chemistry has led to exciting developments in methodological advancements, including photocatalysis, fluorine chemistry, and bioconjugation chemistry.

In this talk, we aim to showcase the potential of flow chemistry and how it can team up with methodological development to take synthetic organic chemistry to the next level. We will highlight the perks of flow chemistry, from improving reaction efficiency to enabling the discovery of new chemical reactions. Our ultimate goal is to inspire chemists to adopt this innovative technology and unlock new possibilities for synthetic organic chemistry.

References:

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POSTER OVERVIEW

No. 1	<u>Light powered mechanically active materials</u> Navneet Kaur Gill / University of Queensland, Brisbane, Australia
No. 2	<u>Harnessing light with carbon quantum dots – bright and colorful fluorescence emissions and photoinduced redox processes driving photocatalysis and antimicrobial functions</u> Ya-Ping Sun / Clemson University, USA
No. 3	<u>Systems controlled by light: A series of thieno[3,2-b]thiophene imines</u> Harry Robson / VŠCHT Prague, Czech Republic
No. 4	<u>Designing new organic photosensitizers for solar light conversion: Applications in dye-sensitized solar cells (DSSCs) and photoelectrochemical cells (DS-PECs)</u> Alessio Dessì / National Council of Research, Sesto Fiorentino, Italy
No. 5	<u>Making the MOST of the photodimerization of 1,4-aryl-substituted anthracenes</u> Till Staschko / University of Siegen, Germany
No. 6	<u>New polymer and macrocyclic hybrid photoswitches: Their synthesis and study</u> Martin Šetek / VŠCHT Prague, Czech Republic
No. 7	<u>A fiber-optic spectroscopic setup for isomerization quantum yield determination</u> Jorn Steen / Uppsala University, Sweden
No. 8	<u>Synthetic advances towards cyclohexaazobenzene for increased storage energy density</u> Silke Müsse / Justus-Liebig-University Gießen, Germany
No. 9	<u>Vis-to-UV photon upconverting porous monoliths</u> Sakura Nakagawa / Kyushu University, Fukuoka, Japan
No. 10	<u>Application of fluorescent organic materials in luminescent solar concentrators (LSCs) and visible light communication (VLC)</u> Massimo Calamante / National Council of Research, Sesto Fiorentino
No. 11	<u>Novel organic dyes for DSSC cells utilizing the intramolecular Förster energy transfer (FRET) to enhance light harvesting</u> Elena Ermini / National Council of Research, Sesto Fiorentino, Italy

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| No. 12 | <u>Functionalisation of gold nanoparticles with arylazopyrazole-modified <i>N</i>-heterocyclic carbene ligands</u>
Dominik Mählmann / University of Münster, Germany |
| No. 13 | <u>Monoaryl-substituted norbornadienes for efficient molecular solar thermal energy storage</u>
Robin Schulte / University of Siegen, Germany |
| No. 14 | <u>Investigation of the photoinduced electron transfer-induced cycloreversion of quadricyclanes to norbornadienes</u>
Julia Hebborn / University of Siegen, Germany |
| No. 15 | <u>Fast T-type photochromism of aza-diarylethenes</u>
Shota Hamatani / Osaka Metropolitan University, Japan |
| No. 16 | <u>Strategies to enhance the half-life of the BOD/TCO photoswitch for improved solar energy storage</u>
Paul Gueben / Universitat Politècnica de Catalunya, Barcelona, Spain |
| No. 17 | <u>Teamwork makes the dream work - Symbiotic lone-pair/π and C-H/π interactions in <i>meta</i>-bis-azobenzenes</u>
Dominic Schatz / Justus-Liebig-University Gießen, Germany |
| No. 18 | <u>Electronic effects on dithienylethene-based organocatalysts</u>
Debashis Majee / National University of Singapore, Singapore |
| No. 19 | <u>Surface tension manipulation with visible light through sensitized disequilibrium of photoswitchable amphiphiles</u>
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| No. 20 | <u>Hemipiperazines as novel peptide-derived molecular photoswitches</u>
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Valentin Schäfer / Karlsruhe Institute of Technology, Germany |

Poster No. 1	Light powered mechanically active materials
	Navneet Kaur Gill , Prof. Paul Burn, Dr. Jos Kistemaker
	University of Queensland, Centre for Organic Photonics & Electronics, Australia

Inspired by biological molecular machines, synthetic chemists have developed nano-scale artificial molecular machines called ‘molecular motors’, which are powered by various forms of energy such as light. The covalently linked sub-components of these machines rotate relative to one another, in response to fuel, in a controlled manner resulting in net work on the surroundings. One of the major goals in this field is the translation of the molecular motion at the nanoscale into an observable phenomenon in the macro world. This can be achieved by harnessing the collective motions of these minute machines by their integration in a polymer system providing responsive materials triggered by light. This project focuses on the development of such light activated polymeric materials, which have the potential for application in fields ranging from medical sciences, soft robotics, chemical catalysis, sensing, and self-healing polymers. This presentation will illustrate the synthesis of a novel molecular motor, and describe its intriguing and unexpected photochemical behaviour, which is found to be dependent on its structural properties. I will show how structural modification of the molecular motor plays a crucial role in its performance. This presentation will further describe the incorporation of the molecular motors into a polymer matrix to develop an active material that will convert light energy into macroscopic changes.

Poster No. 2	Harnessing light with carbon quantum dots – bright and colorful fluorescence emissions and photoinduced redox processes driving photocatalysis and antimicrobial functions
	Ya-Ping Sun
	Clemson University, Department of Chemistry, USA

“Carbon is black!” as average people on the street would describe correctly. Scientifically, the implication of the description is such that carbon is highly effective in harnessing or harvesting light across a broad spectrum including the visible. Interestingly and importantly, however, carbon at the nanoscale may remain black, but can also become a colorful material. In fact, small carbon nanoparticles (CNPs), representing the nanoscale carbon allotrope at the zero-dimension, can be made into a stable solvent dispersion to absorb visible light in a

concentration dependent fashion, not only colorful but also with some weak luminescence emissions. The photoluminescence could be enhanced by orders of magnitude upon the nanoparticle surface being effectively passivated via organic functionalization, namely the formation of carbon “quantum” dots or carbon dots (CDots), which are defined as surface functionalized CNPs. CDots as a new class of photoactive carbon nanomaterials, analogous to and/or competing with the conventional semiconductor quantum dots (QDs), have been developed and studied in our laboratory and by many others for their serving as high-performance yet nontoxic fluorescence agents for bioimaging in vitro and in vivo, as emitting materials in LEDs and other optoelectronic systems, and as efficient photocatalysts for some challenging reactions such as the photocatalytic conversion of carbon dioxide, and also for their highly potent light-activated antimicrobial functions. Highlighted in this presentation are the structures and light-driven properties of CDots and some of their representative applications. Also discussed are the challenges and opportunities in the rapidly advancing and expanding research field of CDots.

Poster**Systems controlled by light: A series of thieno[3,2-b]thiophene imines****No. 3****Harry Robson, Petr Kovaříček**

VŠCHT Prague, Czech Republic

Within the growing field of systems chemistry, it is desirable to be able to control systems of chemical reactions by methods which do not permanently change a systems composition. Here two systems will be presented each with 3-thieno[3,2-b]thiophene imines in the presence of their corresponding amines. The imine systems will be shown to have absorption dependent on the push pull character of the CT state formed, and will be further shown to have controllable composition. Both light and heat will be shown to control the composition at high (10 mM) concentrations. Data will be presented that such a change is reversible, and may be controlled at will, although the change does not seem to depend on which component is excited, suspected due to energy transfer. Equilibration will be shown to occur readily within days, and significant light control noticeable within 10 seconds of minutes. The potential mechanisms for the process will also be explored, supported by ground and excited state calculations.

Poster No. 4	Designing new organic photosensitizers for solar light conversion: Applications in dye-sensitized solar cells (DSSCs) and photoelectrochemical cells (DS-PECs)
	Alessio Dessi^a, D. Franchi^a, G. Reginato^a, M. Calamante^{a, b}, L. Zani^a, A. Mordini^{a, b}
	^a National Council of Research, Institute of Chemistry of Organometallic Compounds (CNR-ICCOM) Sesto Fiorentino, Italy ^b University of Florence, Department of Chemistry "U. Schiff", Sesto Fiorentino, Italy

Nowadays, finding sustainable energy systems is a mandatory research topic to limit global warming and slow the projected rise in CO₂ emissions. Great expectancy is placed on solar energy because it is practically inexhaustible, free, and well-distributed over the world. For this reason, many different photovoltaic technologies exploit solar energy to produce electric current or eco-friendly fuels such as hydrogen.[1] Most photovoltaic systems use small organic molecules as the photoactive material because of their unique optical and electrochemical properties, which can be finely tuned through a balanced modification of the structure and skillful employment of organometallic chemistry and catalysis.

In the last years, we selected several organic chromophores (Figure 1), such as dithieno[3,2-b:2',3'-d]pyrrole (**DTP**),[2] dithieno[3,2-b:2',3'-d]silole (**DTS**),[3] benzo[1,2-b:4,5-b']dithiophene 1,1,5,5-tetraoxide (**to-BDT**), and thieno[3,4-b]thiophene (**ProTT**), and installed them in organic D-A- π -A structures able to anchor on TiO₂-based electrodes. When possible, the dyes were synthesized employing Pd-catalyzed direct arylation reactions to reduce the number of both synthetic and purification steps and the amount of total waste. Depending on the selected chromophore and the proper donor/acceptor moieties, the dyes showed complementary optical properties covering all the visible spectrum and different redox potentials, thanks to which they successfully found applications in different technologies, such as the Dye-Sensitized Solar Cells (DSSCs) and the Dye-Sensitized Photoelectrochemical Cells (DS-PECs) for the conversion of solar energy into electricity and hydrogen, respectively.

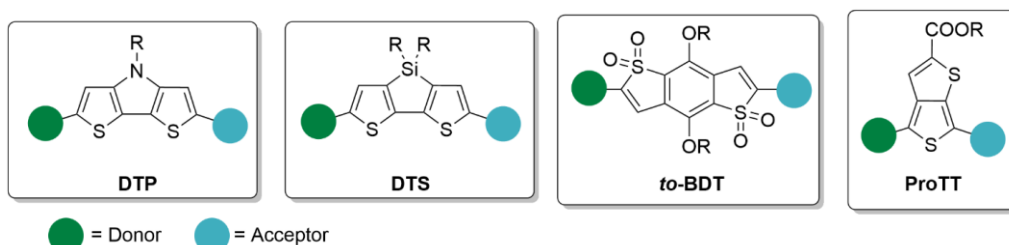


Figure 1: Structures of **DTP**, **DTS**, **to-BDT**, and **ProTT** chromophores.

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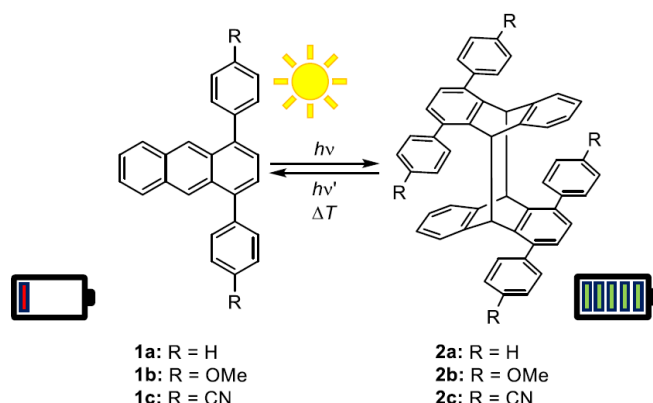
Poster
No. 5

Making the MOST of the photodimerization of 1,4-aryl-substituted anthracenes

Till Staschko^a, R. Schulte^a, S. Afflerbach^b, C. Pritzel^a, H. Ihmels^a
^aUniversity of Siegen, Department of Chemistry-Biology, and Center of Micro- and Nanochemistry and (Bio-)Technology (Cμ), Germany

^bTechnical University of Berlin, Chair of Thermal and Thermochemical Energy Storage, Germany

To reduce the excessive use of fossil fuels and still meet the world's rising energy needs, it is imperative to investigate the efficient and sustainable utilization of green energy sources such as the sun. Sunlight can be converted and stored as chemical energy in molecular solar thermal energy materials (MOST) and released as heat later on demand.[1] In this context, the well-established dimerization of anthracene has experienced a renaissance as a potential MOST material in recent years because of its favorable photochemical and photophysical properties.[2] Herein, we present our studies on novel anthracene derivatives that were readily synthesized that shows some favorable properties as MOST materials. These properties include a pronounced absorption within the range of visible light, high chemical stability of the dimer, high quantum efficiency of the dimerization, and an easily induced cycloreversion to release the stored energy. The 1,4-diaryl-substituted anthracenes **1a–c** contain electron donor and acceptor functionalities, which induce stronger bathochromic shifts with absorption onsets starting at 425 nm. Photocycloaddition reactions occur for every synthesized derivative with excitation wavelengths of <420 nm and even with sunlight and leads regioselectively to the head-to-tail dimers in every case. The cycloreversion reaction can be induced by irradiation with <300 nm light or by heating to 195–270 °C.


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Poster
No. 6

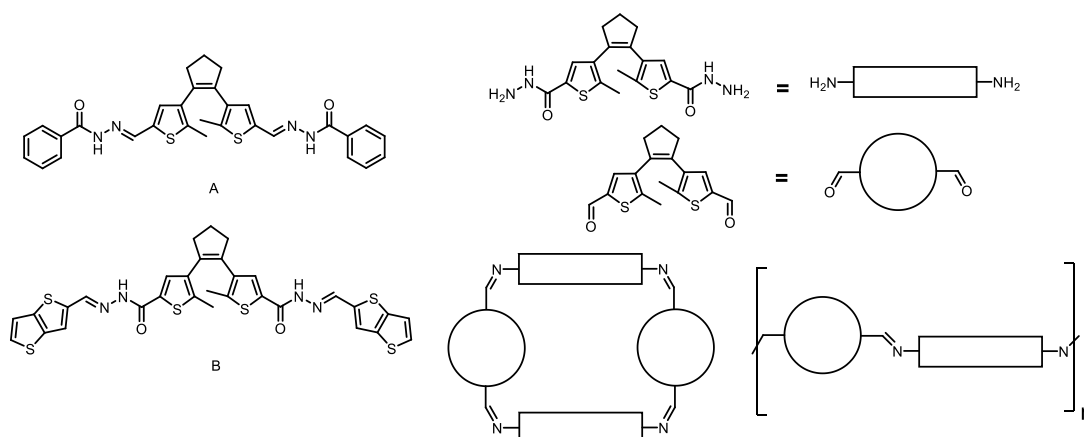
New polymer and macrocyclic hybrid photoswitches: Their synthesis and study

Martin Šetek, Petr Kovaříček

VŠCHT Prague, Czech Republic

New type of hybrid photoswitches combines C=N double bond of acylhydrazones and opening of bis(thienyl)ethenes. Acylhydrazone photoswitches isomerize upon irradiation around the C=N bond to change the configuration of the double bond (*E/Z*). On the other hand, bis(thienyl)ethene photoswitches can change between the open-ring isomer and closed-ring isomer. A particularly interesting feature of acylhydrazones is the formation of radicals after irradiation with light. The presence of unpaired electron density was confirmed by electron paramagnetic resonance (EPR) experiments. The combination of these photoswitchable components results with a new structural motif which could enable the achievement of two localized radicals on thiophene rings. Additionally, if we include the above-mentioned structural motif into a polymeric or macrocyclic structure we can expand the system to further light-tunable properties.

We will present our work involving a multistep synthesis of the two new hybrid photoswitches and a spectroscopic study of behavior upon irradiation and also a synthesis of polymer and macrocyclic hybrid photoswitches. It is possible to use a single wavelength to isomerize all of the photochromes there or back at the same time, but more interestingly we are also able to perform preferential photoinduced isomerization of C=N bond while the bis(thienyl)ethene ring remains closed. Besides exquisite photoswitching in solution, these derivatives also show the isomerization in solid state. We will also demonstrate the application of these new photoswitches as catalysts.


Scheme 1: Hybrid photoswitches.

Poster

No. 7

A fiber-optic spectroscopic setup for isomerization quantum yield determinationAnouk Volker^{a,b}, **Jorn Steen**^a, and Stefano Crespi^a^aUppsala University, Department of Chemistry, Sweden^bUniversity of Groningen, Faculty of Science and Engineering, The Netherlands

We report a simple spectroscopic setup for the determination of isomerization quantum yields built from commercially available optical elements which can be replicated at moderate financial costs.[1] The setup combines fiber-coupled LEDs, a commercially calibrated thermopile detector for direct determination of the power, and a fiber-coupled UV–vis spectrometer. Furthermore, a temperature-controlled cuvette holder and simultaneous UV–vis absorption spectroscopy make this setup suitable for a wide range of photochemical switches, including those with relatively fast thermal back isomerization.

We have demonstrated the validity of our setup by determining the quantum yield of the prototypical photoswitch azobenzene at different wavelengths of irradiation. The UV-vis absorption spectra recorded during irradiation, along with the recently re-determined spectrum of *cis*-azobenzene[2] and the experimentally readily obtained spectrum of *trans*-azobenzene, were used to numerically solve the rate equations[3,4] to yield the quantum yields for both forward and backward isomerization. We show that our results are in good agreement with the most recent literature.[5] After discovering, not surprisingly, that the largest source of uncertainty originates from the power measurement, we decided to include this error in the evaluation of the retrieved quantum yields. The resulting overall uncertainty is in the same order of magnitude as for methods using actinometry,[5,6] thus demonstrating the reliability of our method.

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- [2] L. Vetráková *et al.* *Photochem. Photobiol. Sci.* **2017**, *16*, 1749–1756.
- [3] K. Stranius *et al.* *Sci. Rep.* **2017**, *7*, 41145.
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- [6] G. Gauglitz *et al.* *J. Photochem.* **1985**, *30*, 121–125.

Poster

Synthetic advances towards cyclohexaazobenzene for increased storage energy density

No. 8
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Versatile applicability and practicality of molecular solar thermal (MOST) energy systems require targeted molecular tuning.[1,2] Herein, among other properties, the storage energy density plays a crucial role. One approach towards increasing this parameter is lowering the relative molecular weight. For the mostophore azobenzene (AB) this can be realized by fusing several AB-units in a way that they share phenyl rings (Figure 1). In a cyclic arrangement of six *meta*-connected ABs, this reduces the molecular weight by more than 40 %. Moreover, the storage energy might be enhanced by stabilization of the all-*E*-state via intermolecular π -stacking that is only feasible in the presumed flat ground state (Figure 1). Herein, we report our synthetic advances towards macrocycle **1**.

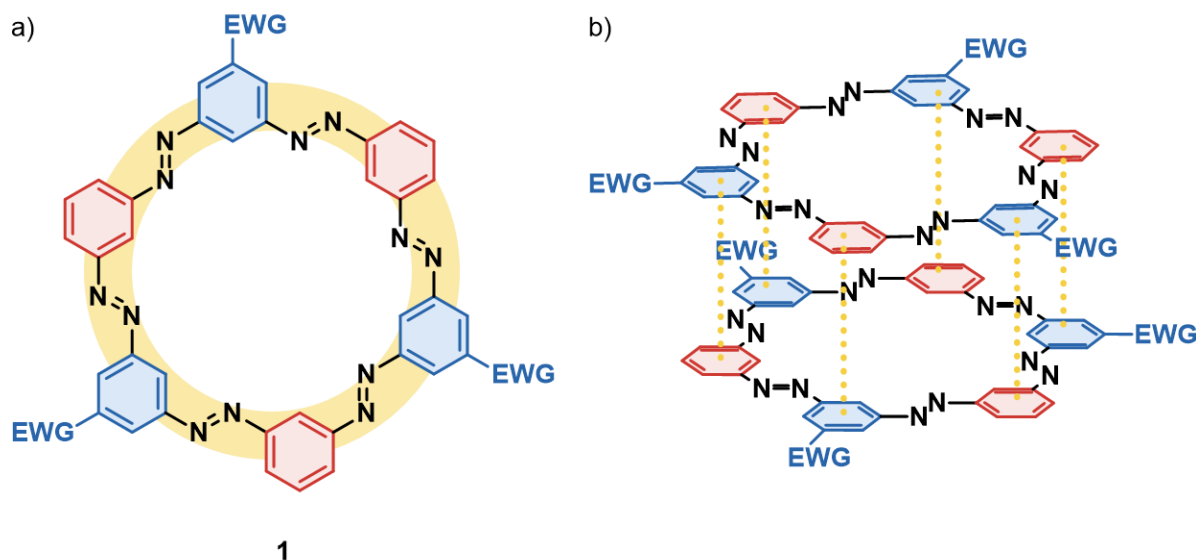


Figure 1: a) Meta-connected cyclohexaazobenzene **1**. b) Intermolecular π -stacking restabilizing the all-*E*-state

References:

- [1] J. Usuba et al. Trends Chem. **2023**, 5, 577.
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- [3] C. Slavov et al. Phys. Chem. Chem. Phys. **2016**, 18, 14795.
- [4] D. Dong et al. ChemPhotoChem **2024**, 8, e202400007.

Poster

No. 9

Vis-to-UV photon upconverting porous monoliths**Sakura Nakagawa^a**, Naoto Matsumoto^a, Masanori Uji^a, Nobuhiro Yanai^{b,c}^aKyushu University, Graduate School of Engineering, Japan^bThe University of Tokyo, Graduate School of Science, Japan^cJapan Science and Technology Agency, CREST, Japan

Ultraviolet (UV) light is useful for driving various photochemical reactions. However, it is not practical due to the limited UV light sources and the low UV transmittance of reaction vessels. In contrast, triplet-triplet annihilation-based photon upconversion (TTA-UC) is an alternative method to generate UV light from visible (Vis) light,[1] which is abundant in sunlight and has high transmittance through reaction vessels. Nonetheless, photoreactions using Vis-to-UV TTA-UC have only been reported in homogeneous solutions and have been desired to develop heterogeneous solid-state materials applicable as photoreactors. Here, we report on the development of a Vis-to-UV TTA-UC porous monolithic material for use in flow photoreactors. The monolith is a porous material with μm -scale cocontinuous structures, which can be synthesized in bulk and is useful as a flow reactor. The monolith was synthesized by polymerization and phase separation of monomer solutions with ketocoumarin derivative (CBDAC) as a donor and naphthalene derivative (TIPS-Nph) as an acceptor. The combination of CBDAC and TIPS-Nph has been reported to exhibit high UC efficiency ($\sim 20\%$) in toluene.[2] The UC emission with the peak top of 375 nm was obtained when a CW laser at 445 nm was irradiated to the UC monoliths. In addition, a low threshold excitation intensity I_{th} of 0.98 mW/cm² was obtained. This value is lower than that of the solar irradiance (~ 1.2 mW/cm²), indicating that it can be driven by an excitation light as low as sunlight. These results suggest that reactions that require UV light can be driven within the monoliths by visible light.

References:

- [1] M. Uji *et al.* *Angew. Chem. Int. Ed.* **2023**, *62*, e202301506.
[2] M. Uji *et al.* *J. Mater. Chem. C*, **2022**, *10*, 4558-4562.

Poster
No. 10

Application of fluorescent organic materials in luminescent solar concentrators (LSCs) and visible light communication (VLC)

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Luminescent solar concentrators (LSCs) are large-area optical devices, capable of harvesting, downshifting and concentrating solar light, thanks to the presence of emitting materials embedded in a polymer matrix.[1] These materials can be used together with silicon-based photovoltaic (PV), to obtain photovoltaic devices able to capture diffuse light. These features with the aesthetic characteristics (colour and shape tunability), allow their use in building-integrated photovoltaics (BIPVs). The same materials could be used as an antenna in visible light communication (VLC), one of the most promising candidates for implementing the future 6G communication paradigm. VLC exploits ordinary LED sources to cast data over the air besides providing for illumination.[2]. In this scenario, exploiting the full spectrum of white LED sources is essential to achieve reliable and efficient VLC links, in the so-called Li-Fi approach.[3]

In order to obtain high-performance LSC devices for both photovoltaic and VLC, a careful study of the materials used for their assembly must be performed, both concerning the selection of the fluorophore and the plastic material in which it is dispersed. We recently synthesized and investigated the properties of a series of organic fluorophores with donor-acceptor-donor (D-A-D) structure, characterized by quinoxaline[4] and benzodithiophene tetraoxide[5] as acceptor cores. The best LSC built with these compounds presented photonic and PV performances close to the state-of-the-art. Moreover, we demonstrated efficient VLC communication using these fluorophores.[6]

References:

- [1] J. Roncali, *Adv. Energy Mater.* **2020**, *10*, 2001907N.
- [2] A. E. Ibhaze *et al.* *JEST*, **2020**, *18*, 100055.
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- [4] C. Papucci *et al.* *J. Mater. Chem. C* **2021**, *9*, 15608–15621.
- [5] M. Bartolini *et al.* *ACS Appl. Energy Mater.* **2023**, *6*, 4862-4880.
- [6] M. Meucci *et al.* *J. Light. Technol.* **2024**, *42*, 2235-2244.

Poster

Novel organic dyes for DSSC cells utilizing the intramolecular Förster energy transfer (FRET) to enhance light harvesting

No. 11

 R. Infantino^a, **Elena Ermini**^a, M. Calamante^{a,b}, A. Dessi^a, D. Franchi^a, G. Reginato^a, L. Zani^a, A. Mordini^{a,b}
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Recently, energy generation has become a crucial scientific and technological issue. Given the increased global demand for energy, there is an urgent need to find new strategies to get energy from renewable sources.[1] In this field, among the new generation of photovoltaic systems, dye-sensitized solar cells (DSSCs) are devices that stand out for their simplicity of fabrication and peculiarities of functioning. For these reasons, such devices have recently received considerable attention with the focus on optimizing their components to improve efficiency.[2]

The same aim can be found in this work in which we present a novel organic photosensitizer (DYAD) designed to improve light-harvesting efficiency (LHE) containing an antenna moiety to enable the well-known Förster Resonance Energy Transfer (FRET) effect, often used to increase the LHE.[3] The novelty of the compound lies in its structure containing a dye with the classical D- π -A sequence used in DSSCs and a covalently bonded antenna (donor). To achieve this purpose, two compounds were designed in order to have complementary spectroscopy properties and they were prepared to be joined together by a "click" reaction as a late-stage connection. Moreover, a model dye was synthesized to verify the increased properties and the FRET effect.

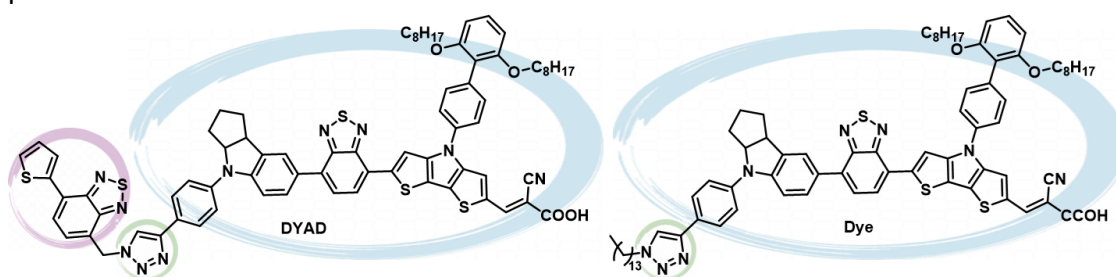


Figure1: Structure of DYAD and model dye.

References:

- [1] D. Gayen *et al.* *Int. J. Environ. Sci. Technol.*, **2024**, *21*, 5285–5310.
 [2] M. Kokkonen *et al.* *J. Mater. Chem. A*, **2021**, *9*, 10527-10545; S. Rahman *et al.* *RSC Adv.*, **2023**, *13*, 19508-19529.
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Poster

Functionalisation of gold nanoparticles with arylazopyrazole-modified *N*-heterocyclic carbene ligands

No. 12

Dominic Mählmann, M. Schrader, A. Nalop, M. Beuel, L. Schlichter, F. Glorius and B. J. Ravoo

University of Münster, Center for Soft Nanoscience, Germany

The properties and applications of gold nanoparticles in medicine, electronics, catalysis and materials are mainly determined by the organic ligands absorbed at the surface. The bond between *N*-heterocyclic carbens (NHC) and gold features special properties e.g. increased conductivity by reducing the work function of gold, and shows great stability and resistance to oxidants, thermal degradation, and organic solvents especially in comparison to thiols. By adding a photoswitchable moiety like arylazopyrazole (AAP) to the NHC ligand, we aim to adjust these properties via external photoresponsive stimuli.

We prepared AAP-NHC functionalised gold nanoparticles using a ligand exchange reaction starting from nanoparticles capped with a weak binding ligand (e.g. oleylamine). The photophysical properties of AAP-NHC capped gold nanoparticles and their behaviour after irradiation with UV and green light were studied using UV/vis measurements. ToF-SIMS and XPS measurements confirmed the formation of the NHC-Au bond.

Using AAP-NHC gold nanoparticles as a molecular ink for dip-pen lithography opens the field to a large variety of applications. By printing a small cluster of nanoparticles between electrodes we hope to create a novel photo responsive electronic network in which the AAP-NHC ligands work as tuneable tunnel barrier between the single gold nanoparticles.

Poster

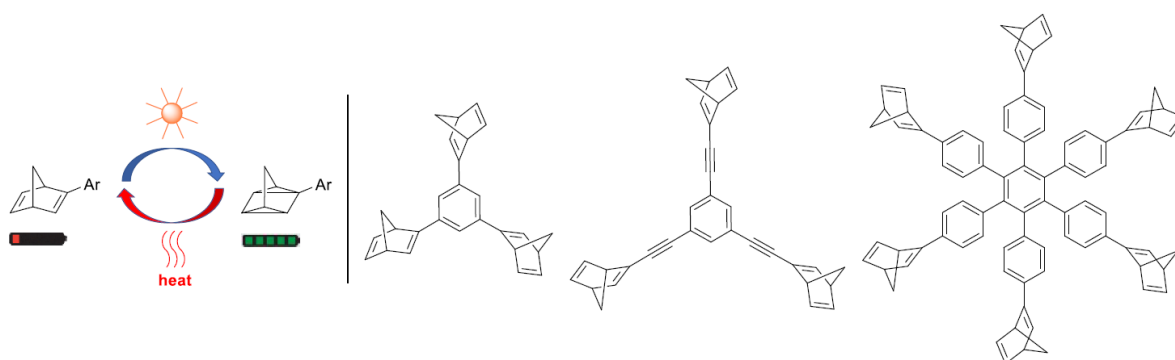
Monoaryl-substituted norbornadienes for efficient molecular solar thermal energy storage

No. 13
Robin Schulte^a, D. Schade^a, T. J. B. Zähringer^b, S. Afflerbach^c, T. Paululat^a, Nico Perez Lopez^b, M. Schmitz^b, C. Kerzig^b, H. Ihmels^a
^aUniversity of Siegen, Department of Chemistry-Biology, Germany

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^cUniversity of the Federal Armed Forces Hamburg, Chair at Helmut Schmidt University, Germany

Molecular solar thermal energy storage (MOST) systems are highly attractive tools to harvest and store (solar) light energy in chemical bonds, i.e., as chemical energy.[1,2] In this study, phenyl- and naphthyl-linked bis-, tris-, tetra- and hexa-norbornadienes are presented as efficient MOST systems with very high energy densities. The substrates were readily available by Suzuki-Miyaura or Sonogashira-Hagihara coupling reactions, and their absorption properties and characteristic parameters for MOST applications were investigated. The norbornadiene derivatives are quantitatively transferred into their corresponding quadricyclanes with quantum yield of nearly 100% in the presence of a triplet sensitizer with visible light. The resulting quadricyclane products have half-lives up to 14 d and very high energy densities of up to 734 KJ/kg.[3] Overall, this class of *monoaryl*-substituted norbornadienes fulfills the necessary criteria for an optimal MOST system and are, therefore, a highly promising basis for the development of materials for efficient solar energy conversion and storage.[3]



Scheme 1: Energy storage and release of monoaryl-substituted norbornadienes.

References:

- [1] Z. Wang *et al.* *Chem. Soc. Rev.* **2022**, *51*, 7313.
- [2] J. Orrego-Hernandez *et al.* *Acc. Chem. Res.* **2020**, *53*, 1478.
- [3] R. Schulte *et al.* *Angew. Chem. Int. Ed.* **2023**, *62*, e202309544.

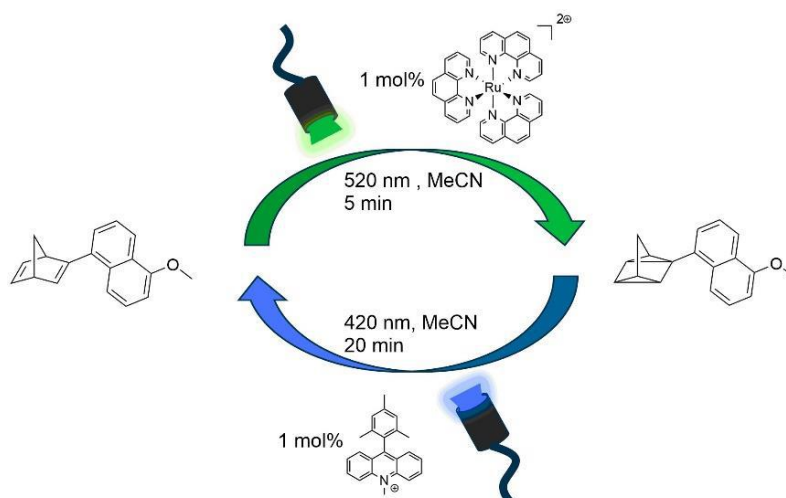
Poster

Investigation of the photoinduced electron transfer-induced cycloreversion of quadricyclanes to norbornadienes

No. 14
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Rising energy demand requires the development of new energy sources. In one approach molecular solar thermal (MOST) materials are employed, which convert and store solar energy as chemical energy. In this context, the photoinduced norbornadiene-quadricyclane system has one of the highest energy storage capabilities.[1-4] For an efficient and controlled release of this energy, a photoinduced back reaction with low-energy light is desirable.[1] In this study, we showed that this goal can be accomplished by the photoinduced electron transfer (PET) reaction of a monoaryl-substituted quadricyclane to the corresponding norbornadiene. Specifically, 5-methoxynaphthyl-norbornadiene was quantitatively converted to the quadricyclane by triplet sensitization with green light ($\lambda = 520$ nm) whereas cycloreversion was induced with several different PET catalysts.



References:

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- [2] E. Franz *et al.* *ChemSusChem* **2022**, *15*, e202201483.
- [3] R. Eschenbacher *et al.* *Nano Energy* **2022**, *95*, 107007.
- [4] A. Gimenez-Gomez *et al.* *Chem. Eur. J.* **2024**, *30*, e202303230.

Poster

**Fast T-type photochromism of
aza-diarylethenes**

No. 15

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Molecular photoswitches that can change their structural geometry and physicochemical properties upon light irradiation have drawn tremendous attention. Especially, diarylethenes have many excellent properties and are expected to be applied in a wide of fields. The photochromism of diarylethenes is based on a 6π electrocyclic reaction. Modulation of the reaction itself may lead to new functions. Therefore, we focused on the 6π aza-electrocyclic reaction. Aza-diarylethenes, in which carbon atom in reaction site of common diarylethenes is replaced with a nitrogen atom, were synthesized and their properties were investigated. When a solution of azadiarylethene was irradiated with light, only the UV-irradiated area became colored, and the colorless state returned immediately after the UV irradiation was stopped. In other words, in contrast to conventional P-type photochromic diarylethenes, whose colored isomer are thermally stable, azadiarylethenes exhibit fast T-type photochromism. Analysis of the thermal back reactivity revealed that the half-life of the reaction is on the order of microseconds to milliseconds. Next, the cause of the fast thermal back reactivity was investigated. By quantum chemical calculations, we focused on the geometric molecular structure change during the thermal back reaction. As a result, it was found that the thermal back reaction of common diarylethenes is based on a conrotatory pathway. Since this is forbidden by the Woodward-Hoffmann rule, the activation barrier for the thermal back reaction becomes large, and the colored isomers become thermally stable. On the other hand, it was found that the thermal back reaction of azadiarylethene is based on a disrotatory pathway, which is allowed by the Woodward-Hoffmann rule. As a result, the activation barrier for the reaction became very small, and the azadiarylethenes showed fast thermal back reactivity.[1]

References:

[1] S. Hamatani, D. Kitagawa and S. Kobatake, *J. Phys. Chem. Lett.*, 2023 14, 8277-8280.

Poster

Strategies to enhance the half-life of the BOD/TCO photoswitch for improved solar energy storage

No. 16
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^bUniversité de Mons (UMONS), Mons, Belgium

In the shift towards an increasing dependence on renewable energy sources, solar energy and its storage play a crucial role in shaping the future of energy management. Molecular solar thermal systems (MOST) are photoswitches capable of undergoing photoisomerization to a higher energy state in which solar energy can be stored. Among the many molecular photoswitches being researched for MOST application, our group has concentrated on the norbornadiene/quadracyclane (NBD/QC) system functionalized with donor/acceptor groups. Another very similar photoswitch that remains quite unexplored is the bicyclooctadiene/tetracyclooctane system (BOD/TCO). This system is expected to offer higher energy storage densities compared to the NBD/QC system but with the drawback of having significantly lower half-lives.[1] BODs also exhibit synthetic challenges as they are prone to degradation into stable retro Diels-Alder byproducts at elevated temperature. This work is aiming at identifying solutions that would enhance the half-life of the BOD/TCO system using different strategies to unleash the full potential of this promising photoswitch.

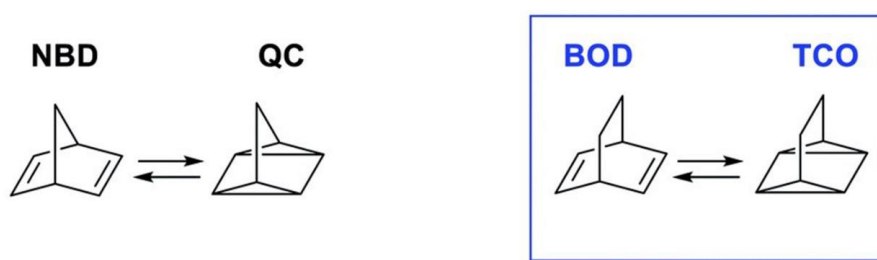


Figure 1: NBD/QC system (left) and BOD/TCO system (right).[2]

References:

- [1] A. Hillers-Bendtsen *et al.* *J. Phys. Chem. A* **2021**, *125*, 10330-10339.
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Poster

Teamwork makes the dream work - Symbiotic lone-pair/ π and $C-H/\pi$ interactions in *meta*-bis-azobenzenes

No. 17
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Unlike pristine azobenzene (AB), azoheteroarenes can show a T-shaped conformation in its (Z)-photoisomer.[1] This configuration lowers the energy of the metastable isomer, and influences the photophysical properties like absorption, half-life and energy storage. Azothiophens can show stabilizing interaction between the sulfur lone-pair and the π -system,[2] while pyrroles and pyrazoles show stabilizing $C-H/\pi$ interactions.[3] By combining both of these properties into a single molecule, we can expect a symbiotic interaction between the electron-donating lone-pair, and the withdrawing $C-H$ interaction. Herein we prepared multiple combinations of lone pair and $C-H$ donating heterocyclic *meta*-bisazobenzenes. Their photophysical properties were studied, and a preliminary trend was observed.

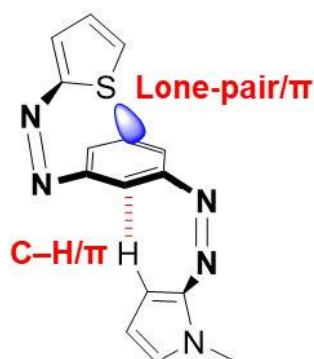


Figure 1: Symbiotic lone-pair/ π and $C-H/\pi$ interactions in a mixed.

References:

- [1] S. Crespi *et al.* *Nat. Chem. Rev.* **2019**, *3*, 133–146.
 [2] J. Calbo *et al.* *J. Am. Chem. Soc.* **2017**, *139*, 1261–1274.
 [3] C. Slavov *et al.* *Angew. Chem. Int. Ed.* **2020**, *59*, 380

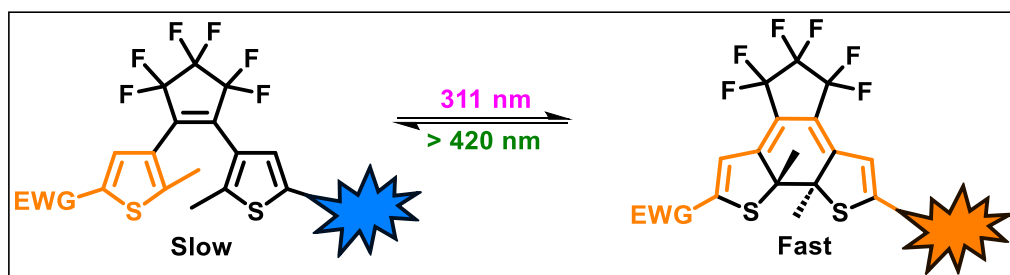
Poster

Electronic effects on dithienylethene-based organocatalysts

No. 18
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National University of Singapore, Chemical and Biomolecular Engineering, Singapore

The advancement of smart catalytic systems has significantly accelerated in recent years, particularly through the use of light as an external stimulus. Photochemically reversible, but thermally-forbidden transformations, however, such as diarylethene 6π -electrocyclization, are still underutilized. In our research, we have designed and synthesized a range of dithienylethene-based thiourea organocatalysts with various electron-donating and electron-withdrawing (EWG) groups. We observed an almost complete conversion from the open to the closed DTE form after exposure to ultraviolet light. This photoisomerization caused a redistribution of electron density, consequently altering the rate of the thiourea-catalysed Michael reaction between (*E*)- β -nitrostyrene and acetylacetone.


Poster

Surface tension manipulation with visible light through sensitized disequilibrium of photoswitchable amphiphiles

No. 19
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Azoarene isomerization lies at the heart of numerous applications from catalysis or energy storage to photopharmacology. While efficient switching between their *E* and *Z* isomers predominantly relies on UV light, a recent study by Klajn and co-workers introduced visible light sensitization of *E* azoarenes and their subsequent isomerization as a tool coined disequilibrium by sensitization under confinement (DESC) to obtain high yields of the *Z* isomer. This host-guest approach is, however, still constrained to minimally substituted azoarenes with limited applicability in advanced molecular systems.

Herein, we expand DESC for the assembly of surfactants at the air–water interface. Leveraging our expertise with photoswitchable amphiphiles, we induce substantial alterations of water’s surface tension through reversible arylazopyrazole isomerization. After studying the binding of charged surfactants to the host, we find that the surface activity differences upon visible light switching for both isomers are comparable to those obtained by UV light excitation. The method is demonstrated on a large concentration range and can be activated using green or red light, depending on the sensitizer chosen. The straightforward implementation of photoswitch sensitization in a complex molecular network showcases how DESC enables the improvement of existing systems and the development of novel applications driven by visible light

Poster**No. 20**

Hemipiperazines as novel peptide-derived molecular photoswitches

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^aKarlsruhe Institute of Technology, Institute of Organic Chemistry, Germany

^bKarlsruhe Institute of Technology, Institute of Biological and Chemical Systems – FMS, Germany

Using light as a trigger to reversibly change the geometry of molecules has gained a lot of interest in recent years, not least because of its high degree of selectivity and orthogonality. Molecules that react upon light illumination with an alteration of their geometry, known as molecular photoswitches, have thus far been employed in a broad range of varying research context, e.g. data storage, material science and energy storage systems. Employing molecular photoswitches in a biochemical context as dynamically addressable active compounds or fluorescent labels has been demonstrated numerous times to be a promising lead for groundbreaking scientific advancement.

One such example was the focal point of our latest studies, which revolved around plinabulin and its previously unknown ability to photo-isomerize and thus reversibly change its anti-mitotic activity by two orders of magnitude. The photochromic motif of plinabulin, which we dubbed “hemipiperazine” (HPI), had thus far not been described. This led us to investigate this new class of molecular photoswitches in more detail. A further minor structural change to plinabulin also led to the discovery of fluorescent molecular photoswitches, which we dubbed “indolo-hemipiperazines” (IndHPis).

Here, we report the in-depth photophysical investigations of HPIs and IndHPis, which have been shown to be water-compatible and able to withstand physiological reductive conditions over multiple switching cycles. Further, HPIs exhibit high selectivity in addressability of either isomer, in some cases even near-quantitative photostationary states, while IndHPis even show

addressability with biocompatible red-light. In some IndHPIs, the luminescence can be modulated in its intensity upon photo-isomerization, which is shown to even be possible inside of living cells.

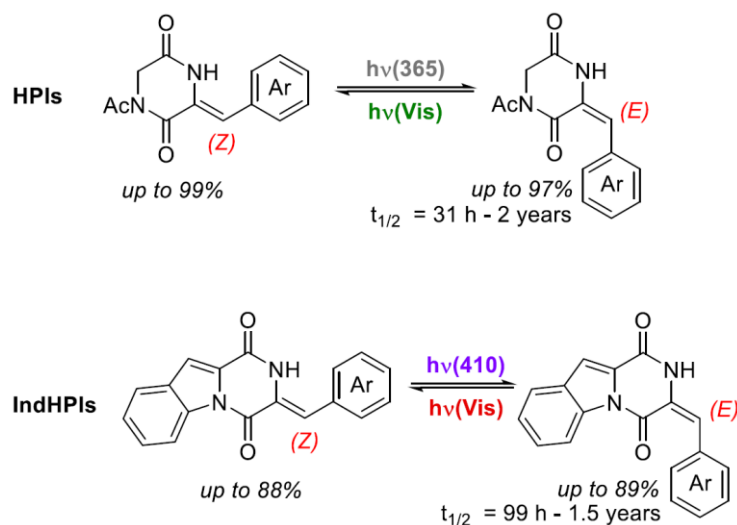


Figure 1: General structural motif of HPIs (top) and IndHPIs (bottom) and outline of their photophysical properties.

References:

- [1] S. Kirchner *et al.* *Nat. Comm.* **2022**, *13*, doi: 10.1038/s41467-022-33750-7.
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Poster

No. 21

Hemipiperazine-based photochromic sensors and nanomaterials

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Our group recently introduced a novel class of molecular photoswitches, known as hemipiperazines (HPI), which are derived from cyclic dipeptides. The photochromic behavior of HPIs arises from the *E/Z*-photoisomerization of an arylidene group linked to a 2,5-diketopiperazine ring. HPIs exhibit several advantageous photophysical properties, such as an extended thermal half-life, significant band separation, and broad applicability, including compatibility with water, the ability to modulate bioactivity with light, and photoswitchable fluorescence.[1–3]

We are currently exploring applications for these novel photoswitches, one of which involves the development of stimuli-responsive smart materials. In this context, we demonstrate that specific HPI derivatives can function as phototunable fluorogenic sensors for metal ions, combining a reversible light response with a metal-induced fluorescence enhancement. For instance, ion-dependent photoisomerization of the ligand allows for the differentiation between metal ions that typically exhibit similar complexation properties. Additionally, it has been shown that these complexes can self-assemble into nanostructures, resulting in intricate multi-stimuli responsive systems.[1] This discovery opens the door to a new class of peptide-derived metal sensors and quantum confined materials. Given the exceptional thermostability, robustness, modular synthesis, and compatibility with polar and aqueous environments, future applications of HPI in other stimuli-responsive molecular architectures are highly promising.

References:

- [1] V. Schäfer *et al.* *Chem. Eur. J.* **2024**, *30*, e202402005.
- [2] S. Kirchner *et al.* *Nat. Commun.* **2022**, *13*, 6066.
- [3] P. Gödtel *et al.* *Chem. Eur. J.* **2023**, *29*, e202204009.