



WOMEN IN SCIENCE

5th Erlangen Symposium

30.09. - 02.10.26

BOOK OF ABSTRACTS

Inspiring
the next generation

Table of Content

Foreword.....	3
Scientific Advisory Committee	4
Organizing Committee.....	5
Administrative Support	8
Advisor	Error! Bookmark not defined.
Funding	9
General Information	11
Transportation.....	12
Detailed Programme	13
Invited Speakers	14
Invited Speaker - FAU Speakers	19
Abstracts.....	20
Invited Speakers	21
Flash Talks.....	36
Poster Abstracts.....	45

Foreword

As members of the Women in Science-Erlangen Symposium Organizing Committee, it gives us immense pleasure to welcome you to the 5th edition of our symposium series at the Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg in Germany.

The Women in Science - 5th Erlangen Symposium has been organized by doctoral students and postdoctoral researchers from the Department of Chemistry and Pharmacy and the Department of Biology at FAU Erlangen-Nürnberg. First conceptualized in 2018, the main goal of this valuable platform is to address gender imbalances – particularly in the field of chemistry – by increasing the visibility of female researchers, fostering a conversation across an international network, and inspiring young scientists.

We are delighted to welcome almost 200 participants from many different career stages to the 5th edition of our Symposium. Over the course of three days, top-notch female scientists from diverse research fields such as physical chemistry, computational chemistry, life sciences, and biology, among many others, will not only deliver their research findings, but they will also showcase their professional careers and personal experiences in academia and/or industry. All participants, from early-stage bachelor students to senior professors, will have the opportunity to establish new network connections and collaborations.

The symposium program includes invited lectures and flash talks, as well as poster and brain-dating sessions. In addition, considerable time will be devoted to discussing diversity and inclusion in the workplace, positive discrimination, and other relevant topics that can be discussed during the brain-dating sessions. While the primary focus of our Symposium is women in science, we would like to emphasize that this event is open to everyone, regardless of gender or status. The goal of all our symposium sessions and activities is to share research ideas and results, promote scientific discussions and new collaborations, and encourage each participant to actively take part in the symposium.

We hope that this symposium will serve as an inclusive and unique platform for fruitful discussions and networking opportunities. We wish you a pleasant and productive stay in Erlangen.

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Funding

The members of the Organizing Committee of WIS26 are grateful for the continuous administrative support from the Department of Chemistry and Pharmacy of the FAU Erlangen-Nürnberg. We would also like to thank the GdCh for providing the poster prize for our symposium.

Supporting research consortia at FAU

We are thankful for the support of the following research consortia at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), funded by the **German Science Foundation** (DFG), through their means for promoting equality, with organizational support from **F³G network** at FAU. Participating consortia are:

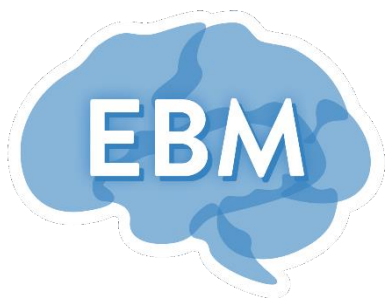
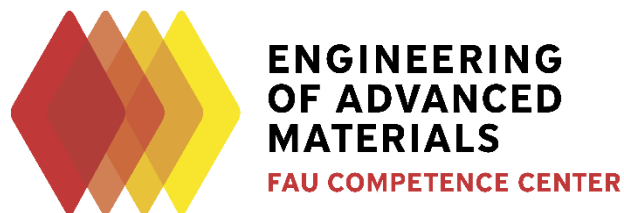
- CRC 1411 – Design of Particulate Products
- CRC 1540 – Exploring Brain Mechanics (EBM)
- CRC 1719 – Next-generation printed semiconductors (ChemPrint)
- RTG 2423 – Fracture across Scales (FRASCAL)
- RTG 2861 – Planar Carbon Lattices (PCL)
- RTG 2950 – Solidification cracks during laser beam welding

Supporting institutions at FAU:

- FAU Competence Center Engineering of Advanced Materials (FAU EAM)
- FAU Womens Representatives
- FAU Profile Center New Materials and Processes (FAU NMP)
- Department Chemistry and Pharmacy, FAU

Support from outside FAU:

- JungesChemieForum (JCF)
- Gesellschaft Deutscher Chemiker (GdCh)



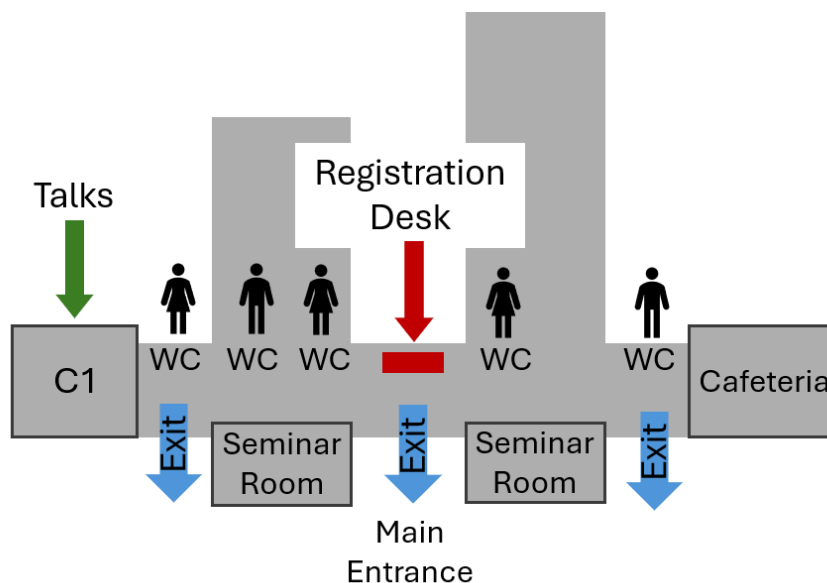
General Information

Conference Site:
Chemikum
Friedrich-Alexander-University-Erlangen-Nuremberg
Süd (South) Campus Nikolaus-Fiebiger-Str. 10
91058 Erlangen



Photo: Staatliches Bauamt Erlangen-Nürnberg

The *Chemikum* building of FAU represents the ideal location for the symposium, housing several of FAU's chemistry departments under its roof. Fully equipped lecture halls ensure the realization of the Symposium in a modern environment. It also offers ample room for the poster session, stimulating and inspiring further discussions. Please see the following map of the Chemikum for details. All lectures will take place in the lecture hall C1. Coffee breaks, lunch, and the poster session will be in and around the seminar rooms. All rooms are located on the ground floor.



Transportation

Airports:

- Airport Nuremberg: to reach Chemikum, take VGN Bus 30 (bus stop with yellow H on the left once you exit the airport) to the "Erlangen Süd" bus stop and then walk 12 minutes down Egerlandstr. (approx. 40 min and 4€) or take a taxi (approx. 30 min and 40-50 €)
- Airport München and Airport Frankfurt: (approx. 3 hours by train)

Public Transport:

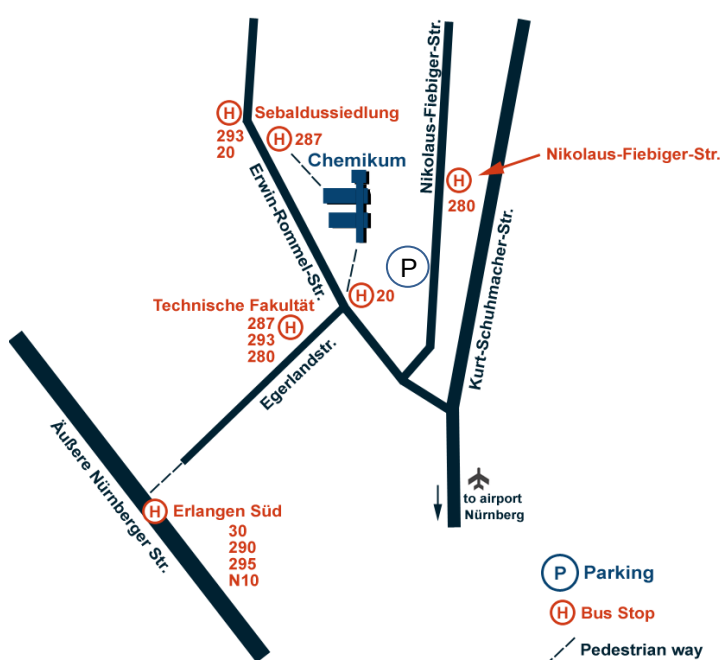
Bus tickets can be purchased on the bus with cash or with debit/credit cards in the VGN app; train tickets can be purchased at one of the automatic machines at the station, on the VGN app, or the Deutsche Bahn (DB) app.

From Nuremberg: take the VGN Bus 30 to the bus stop "Erlangen Süd" or a local train to the main Erlangen train station and one of the buses below

Train: there are four train stations within Erlangen; the main train station is called "Erlangen Bahnstation" on Bahnhofplatz, which is considered city center

Bus: from main train station "Erlangen Bahnstation", the following buses depart regularly:

- Bus 287 direction "Sebaldussiedlung," stop at "Technische Fakultät", then approx. 5 min walk to Chemikum
- Bus 293 direction "Bruck Bahnhof", stop at "Sebaldussiedlung", then approx. 3 min walk to Chemikum
- Bus 295 direction "Tennenlohe", stop at "Erlangen Süd", then approx. 12 min walk to Chemikum



Detailed Programme

Wednesday		
	9:00 - 10:00	Registration
	10:00 - 10:30	Welcome Speech: Ingrid Span
Session 1: Julien Bachmann	10:30 - 11:10	Dorothea Wisser <i>Solid-state NMR Spectroscopy for Molecular Level Understanding of Material Structures</i>
	11:10 - 11:50	Swetlana Schauermann <i>Molecular systems for reversible hydrogen storage: atomistic-level insights</i>
	11:50 - 12:00	Flash talk: Kira Mikulinskaya <i>STM study of the Nucleation of Tris(dimethylamido)antimony on CoO Nanoislands</i>
	12:00 - 13:00	Lunch Break
Session 2: Ilaria Bettin	13:00 - 14:00	Flashtalk Session
		Kleopatra Papagrigoriou <i>Probing fluorescence lifetimes of quantum dots in the gas phase</i>
		Hemlata Agarwala <i>Metal-Ligand Electronics Dictate Divergent Photoredox Pathways for CO₂-to-CO Conversion from Dilute and Impure CO₂ Streams</i>
		Alina Petrovskaja <i>Molybdenum octahedral clusters and Vanadium polyoxometalates as photoinitiators and cross-linkers for functional PEGDA hydrogels with antibacterial properties</i>
Session 3: Esther Zanin	14:00 - 15:30	Helena Schwarz <i>Engineering the Implant–Bone Interface: Mesoporous Bioactive Glass Nanoparticle-Enriched Coatings on β-Titanium Alloys</i>
		Daria Berdnikova <i>Aurones: from photoswitches to RNA binders and solid-state emitters</i>
		Diptiprava Sahoo <i>All-Photonic Yellow-Red-Blue-Green Orthogonal Photoswitching or Rewritable Four-Color 2D and 3D Displays and Optical Memories</i>
		Coffee Break + Brain dating
Session 3: Esther Zanin	15:30 - 16:10	Petra Imhof <i>From Chemistry to Bio-Physics and back</i>
	16:10 - 16:50	Nadja Simeth-Crespi <i>Light-Responsive Tools for Biological Systems</i>
	16:50 - 17:00	Flash talk: Hannah Buttkus <i>Molecular-Level Insights into the Catalytic Activity of Hexafluoroisopropanol probed by Gas-Phase IR Spectroscopy</i>
	19:00	Speakers' Dinner (upon invitation)

Thursday

Session 4: Cláudia Vilhena	9:00 - 9:40	Dorothea Kaufmann <i>Building the Table Together: How Women in Science Can Shape Structures for True Equality</i>
	9:40 - 10:20	Gesine Born <i>Missing pictures</i>
Session 5: Lisa Pecher	10:20 - 10:50	Coffee Break
	10:50 - 11:30	Christine-Maria Horejs <i>Shaping Scientific Conversations: An Editor's View</i>
	11:30 - 12:10	Katharina Kohse-Höinghaus <i>Burning for science: of endangered species, bad moms, and female pioneers</i>
Session 6: Vipul Kumar Ambasta	12:10 - 13:00	Lunch Break
	13:00 - 14:00	Gesine Born: Workshop <i>Show Me a Female Scientist: On Images, Stereotypes, and AI</i>
	14:00 - 14:40	Dandan Gao <i>Advanced Electrocatalytic Approaches for Sustainable Chemistry and Mechanistic Studies</i>
Session 7: Carolin Müller	14:40 - 15:40	Coffee Break + Brain dating
	15:40 - 16:20	Jannika Lauth <i>Colloidal 2D Semiconductor Nanocrystals en Route to Photonics</i>
	16:20 - 17:00	Melanie Schnell <i>Molecular interactions revealed with rotational spectroscopy: Structure, dynamics, and chirality</i>
	17:00 - 19:00	Poster session and Finger Food

Friday

Session 8: Martina Hartinger	09:00 - 09:40	Kasia Pernal <i>TBD</i>
	09:40 - 10:20	Giuliana Giunta <i>Advancing Soft Matter Science Through Digitalization and Multiscale Modelling</i>
Session 9: Ingrid Span	10:20 - 10:50	Coffee Break
	10:50 - 11:30	TBD
	11:30 - 12:10	Sofia Pauleta <i>Metalloenzyme s Supporting Bacterial Survival During Infection: Novel Targets Against Antibiotic Resistance</i>
	12:10 - 12:30	Award Ceremony and Closing Remarks
	12:30	Lunch and Farewell

Invited Speakers

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Abstracts

Invited Speakers

Missing Pictures

Gesine Born^{1*}

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Some female scientists left behind no portraits—no photographs, no paintings, no traces in the collective visual memory. “Missing Pictures” uses AI to address precisely this gap: not to invent history, but to open up a space of possibility—in the minds of viewers, within institutions, and in the culture of remembrance. What happens when we begin to imagine who might have been there?

Show Me a Female Scientist: On Images, Stereotypes, and AI

Gesine Born^{1*}

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How can we make images in science more engaging and innovative, and who actually becomes visible when we talk about science?

This talk takes a closer look: we analyse images of science in general, and in particular for stereotypical representations, and ask which people, bodies and perspectives are systematically missing.

There is a particular focus on AI-generated images: what does artificial intelligence reproduce – and why? The built-in bias of the systems itself becomes a topic of discussion.

Anyone who wishes to can participate alongside the talk: at several points, there will be opportunities to test the observations presented using your own AI-generated images and to share the results with the group. However, this is not compulsory. The examples work just as well for those simply watching.

Advanced Electrocatalytic Approaches for Sustainable Chemistry and Mechanistic Studies

Dandan Gao^{1*}

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The research program of my group is dedicated to the development of efficient nanomaterials for sustainable energy conversion reactions, in particular using renewable electricity as the primary green energy source. The central starting point is to deploy technically relevant base metals to upgrade low-value natural feedstocks or even environmental pollutants under continuous operation, leading to scalable production of industrially more important chemicals, intermediates and fuels. The program will investigate the studied reactions/systems from the molecular level through to the reactor level using advanced *in situ/operando* physico-chemical methods. Complementarily, the established collaboration with theoretical chemists will provide substantial insights at the atomic level. This is expected to deliver thus-far unavailable understanding of the mechanisms at different length- and time-scales which govern catalytic performance, thus facilitating knowledge-based development of future-improved energy conversion/storage and water purification systems.

Advancing Soft Matter Science Through Digitalization and Multiscale Modelling

Giuliana Giunta¹

¹BASF SE, 67063 Ludwigshafen am Rhein, Germany

In my presentation, I will outline my professional journeys, highlight my role as Senior Specialist Digitalization in R&D at BASF, and discuss how digital technologies are advancing soft matter development. I will explain how computational and multiscale simulations streamline product design and optimization by reducing experiments, screening formulations, and uncovering key molecular interactions. Case studies will illustrate our approach to developing sustainable, high-performance formulations. My aim is to share both scientific insights and experiences to encourage researchers at various career stages.

Shaping Scientific Conversations: An Editor's View

Christine-Maria Horejs^{1,*}

¹Springer Nature, Berlin, Germany

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Publishing is at the heart of scientific progress. However, the pathways into editorial work are often less visible. In this talk, I will offer an inside look at scientific publishing, from the daily work of shaping manuscripts to the broader role editors play in curating scientific conversations and guiding the development of research fields. I will discuss what editors look for in submissions, how decisions are made, and how we balance scientific rigor, innovation and clarity. I will also share insights into my editorial career, and what a transition from research to publishing can look like.

Building the Table Together: How Women in Science Can Shape Structures for True Equality

Dorothea Kaufmann^{1,*}

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As a scientist, local politician, and mentor, I am driven by the conviction that gender equality in science is not just about securing a seat at the table - it is about collectively building that table. Drawing from my interdisciplinary experiences, I will explore how women can actively co-create the frameworks, networks, and policies that foster inclusive environments. My talk will highlight concrete strategies for dismantling systemic barriers, from grassroots mentoring to institutional advocacy, and emphasize the power of collaboration across sectors. By sharing personal insights and lessons learned, I aim to inspire a dialogue on how we can move beyond symbolic representation to structural transformation. Together, we can build a future where women not only participate in science but lead its evolution.

Burning for science: of endangered species, bad moms, and female pioneers

Katharina Kohse-Höinghaus^{1,*}

¹Departement of Chemistry, Bielefeld University, Germany

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Careers in science, technology, engineering, and mathematics (STEM) are often still considered to be less attractive to women. Already from a young age, a talent for such subjects is more frequently attributed to boys than to girls, and social influences within families and at schools continue to affect career choices. Success and growth in an academic environment of STEM disciplines may still be perceived as more difficult for women, depending on local factors, self-concept, and available support structures.

Looking back on my own career, I will introduce some of my research interests and reflect on some of the factors at different stages that have influenced my career in an academic context over the past 50 years. The audience will be encouraged to identify aspects for further thought and discussion.

Colloidal 2D Semiconductor Nanocrystals en Route to Photonics

Jannika Lauth^{1,2,*}

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²Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, 30167 Hannover, Germany

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The direct wet-chemical synthesis of 2D nanomaterials yields materials with strong excitonic contribution already at room temperature and bright photoluminescence, which is favored in photonics. In my talk I will touch on recent examples on how we tailor 2D nanocrystals with efficient optical gain properties, photoluminescence at fiber-optics relevant telecom wavelengths for ensemble and toward single photon emitting properties. We characterize the light-matter interactions in colloidal 2D nanocrystals with a highly accurate stopwatch – by light itself! Following the generation, fate and recombination of excited states in the materials is one of the key features in driving and explaining their photophysical processes.

We combine our unique wet-chemistry – spectroscopy feedback loop to unravel photoexcitation-induced dynamics in highly diverse systems, which range from molecular over plasmonic to semiconducting 2D nanomaterials on their way to innovative photonics.

Additionally to scientific results, I will touch upon some – hopefully interesting – personal experiences during my career journey.

Metalloenzymes Supporting Bacterial Survival During Infection: Novel Targets Against Antibiotic Resistance

Ricardo N. S. Oliveira¹, Anita Gonçalves¹, Daniela S. Barreiro¹, Pedro Bragança¹, Sofia R. Pauleta^{1,*}

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The emergence of pathogenic bacterial strains resistant to most available antibiotics is a major public health concern. Consequently, there is an urgent need to develop new antimicrobial compounds and identify novel bacterial molecular systems that can serve as selective therapeutic targets. Our research focuses on metalloenzymes involved in anaerobic respiration and copper detoxification, processes that promote bacterial survival during infection. We combine structural, biochemical and kinetic approaches to elucidate the catalytic mechanisms, structure-function relationships and protein-protein interactions of these enzymes, providing insights into their roles in bacterial physiology and pathogenicity. Molecular systems from *Neisseria gonorrhoeae* and *Escherichia coli* will be presented.[1–6]

References

- [1] D.S. Barreiro, R.N.S. Oliveira, S.R. Pauleta, *Coord. Chem. Rev.* **2023**, 485, 215114.
- [2] C.S. Nóbrega, A.L. Carvalho, M.J. Romão, S.R. Pauleta, *Int. J. Mol. Sci.* **2023**, 24, 6246.
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- [4] P.M. Bragança, D.S. Barreiro, M.S.P. Carepo, S.R. Pauleta, *J. Inorg. Biochem.* **2026**, 276, 113164.
- [5] C.S. Nóbrega, B. Devreese, S.R. Pauleta, *Biochem. Biophys. Acta.* **2018**, 1859, 411.
- [6] R.N.S Oliveira, S.R.M.M. de Aguiar, S.R. Pauleta, *Molecules* **2023**, 28, 4598.

Electron Density and Reduced Density Matrices as Tools for the Quantum Description and Prediction of Molecular Properties

Katarzyna Pernal^{1,*}

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An accurate description of many-electron systems in quantum chemistry generally requires solving the Schrödinger equation and determining the full wavefunction. However, the wavefunction is an extremely complex object, difficult both to compute and to interpret. It has long been known, however, that much of the key information about electronic matter, and molecules in particular, can be obtained from considerably simpler quantities: the electron density and the one- and two-electron reduced density matrices.

In the first part of the seminar, I will introduce these concepts and discuss their relationship to the full wavefunction. I will also present modern computational methods that enable the electronic structure of molecules to be determined without directly referring to the wavefunction, using only reduced quantities.

In the second part, I will show how reduced density matrices, used in combination with an approximate wavefunction, can be employed to predict excited-state energies and molecular properties such

as electric polarizability. I will also discuss a hybrid approach to quantum computing, in which molecular energies are determined from density matrices obtained from calculations performed on a quantum computer.

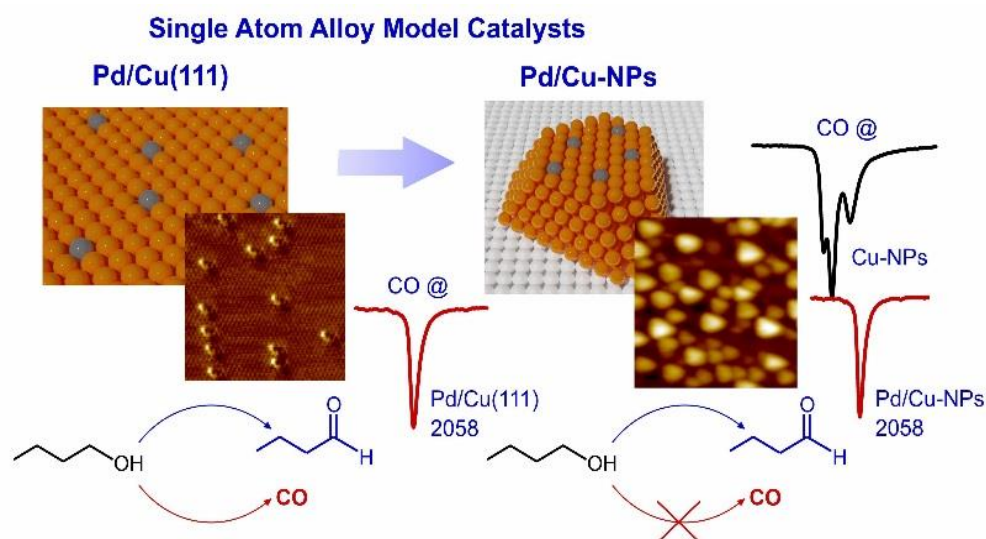
Molecular systems for reversible hydrogen storage: atomistic-level insights

Swetlana Schauermann^{1,*}

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Heterogeneous catalysts based on bimetallic single atom alloys (SAA) play a significant role in numerous technical processes. The fundamental working principles of these systems, however, remain poorly understood, especially the aspects related to the nanoscopic nature of bimetallic particles and the associated structure-reactivity relationships. In this study, we developed well-defined SAA catalysts consisting of Pd atomically dispersed in Cu nanoparticles prepared under ultra-high vacuum (UHV) conditions on model $\text{Al}_2\text{O}_3/\text{NiAl}(110)$ support. Employing a unique combination of surface sensitive techniques – scanning tunneling microscopy (STM), infrared reflection absorption spectroscopy (IRAS), molecular beam techniques – and density functional theory (DFT) calculations, we performed detailed structural characterization of these systems at the microscopic level and linked their structural properties to the catalytic performance. The developed Pd/Cu nanostructured systems show an outstanding catalytic performance in selective dehydrogenation of butanol and exhibit 100 % selectivity toward butanal over a broad range of Pd loadings – the property that cannot be reproduced employing simplified single crystalline Pd/Cu(111) counterparts.¹ The developed approach for preparation and characterization of these nanostructured SAA-catalysts lays a foundation for further fundamental-level catalytic studies on this important class of materials and their rational design for practical applications.



[1] P. A. Fredersdorff (Haugg), J. Smyczek, C. Schröder, P. Fröhlich, P. Kohlmorgen, S. Appelfeller, K. Neyman*, S. Schauermann* *Angew. Chem. Int. Edit.* (2026), 65, e21885 (DOI: [10.1002/anie.202521885](https://doi.org/10.1002/anie.202521885))

Molecular interactions revealed with rotational spectroscopy: Structure, dynamics, and chirality

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Rotational spectroscopy is a coherence technique known to determine the structures of molecules and molecular complexes in the gas phase in great detail – ranging from fundamental topics like proton transfer in microsolvated acids to molecular recognition and astrochemistry. The structural information that can be deduced from the spectroscopic data provides an unprecedented molecular view on chemical processes, such as solvation and molecular recognition, governed by a tight interplay between hydrogen bonding and dispersion.

One fascinating example where intermolecular interactions can shape molecular structures concerns chirality induction, as in the case of achiral tetraethyllead interacting with chiral trifluoromethyloxirane. In this complex, the latter induces a handedness in the highly flexible, initially achiral tetraethyllead compound. This chirality induction causes an increased predicted energy difference between the two enantiomers of this complex due to parity violation.

Rotational spectroscopy has also developed into an interesting tool to investigate and control the handedness of chiral molecules, using a microwave three-wave mixing approach and its extension to enantiomer-selective population transfer. Here, I will report how this technique can be used to investigate tunneling between enantiomers hindered by a rather low barrier.

Light-Responsive Tools for Biological Systems

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Organic chromophores are the foundation for developing light-responsive compounds that enable control over bioactive functions and site-specific labelling reactions in opto-chemical biology and photopharmacology. These light-responsive molecules include photoswitches, photocages, and click reagents, and are often appended onto a bioactive molecule or structurally merged with it to couple the light-mediated structural change to a change in bioactive function or site-specific labelling reactions.

To achieve optimal performance in biological systems, the chromophore structure and properties need to match the requirements for photopharmacology, such as fast and clean conversions with pronounced structural changes. This can be achieved through substituent design and optimization of the chromophore core structure, and is constrained by considerations of the intended application.

We will present approaches for designing and optimizing different types of chromophores for opto-chemical biology and photopharmacology. We will showcase both small molecule modulation and biomolecule conjugates, for example, using azobenzene-based photoswitches for controlling protein function, and the development of photocages for site-specific labelling of biomolecules. Our work aims to provide a deeper understanding of the design principles for light-responsive chromophores and their potential applications in opto-chemical biology and photopharmacology as well as challenges and opportunities of the field.

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From Chemistry to Bio-Physics and back

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As a computational chemist, my research evolves around molecules – what they look like and how they undergo changes of different scales: small geometry changes upon photo-excitation, vibrations, conformational transitions (per se), or as a response to binding (non-covalently) to another molecule breaking and forming of bonds, i.e. creating new molecules. As a computational chemist, I study molecules and their properties and behaviour by computational means, i.e. by simulations.

The types of change/transition and the associated time scale(s) pose different challenges to the feasibility of the simulation, leading to sacrifices in accuracy (empirical potentials instead of first-principles calculations), in limitations of affordable simulated time (only a few ps or using static calculations), or both. In this presentation, I will show examples of molecular simulations which, despite all limitations, afforded us to gain atomic-level insight into the geometric response to photo-excitation, enzyme specificity, chemical reactivity, and combinations thereof.

Solid-state NMR Spectroscopy for Molecular Level Understanding of Material Structures

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Solid-state NMR spectroscopy is one of the most powerful techniques for atomic-level characterization of functional materials, enabling a molecular understanding which is essential for knowledge-based optimization. The solid-state NMR group of Dr. Dorothea Wisser at the Erlangen Center for Interface Research and Catalysis (ECRC), FAU Erlangen-Nürnberg, develops new Magic Angle Spinning (MAS) NMR methods to investigate surfaces and interfaces in modern materials for applications in catalysis, optoelectronics, and separation. A focus lies on in situ and operando MAS NMR techniques to enable real-time observation of catalytic reactions under realistic operating conditions, and in particular photoinduced processes via light irradiation inside a spinning MAS rotor. Current research project cover Supported Ionic Liquid Phase catalysts, porous and functionalized silica materials, nanoparticles as well as thin films of semiconductors and perovskites.

Flash Talks

Metal-Ligand Electronics Dictate Divergent Photoredox Pathways for CO₂-to-CO Conversion from Dilute and Impure CO₂ Streams

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The management and valorization of CO₂ is a critical, contemporary challenge with significant implications for academia, industry, policymakers, and public organizations^[1]. Deciphering the underlying mechanisms of catalyzed reactions are pivotal to optimizing catalytic performance and selectivity. To this end, my talk will delve into some recent catalysts that we have developed and are studying for CO₂ reduction, their structural and functional properties, and the catalytic pathways that these catalysts navigate. Integrating computational modelling and experimental investigations, such as *in situ* spectroscopy and photoluminescence quenching, have uncovered how features such as optimum structural flexibility, electronic coordination, solvation effects and second coordination sphere interactions synergistically lower energy barriers and enhance catalytic efficiency^[2-5].

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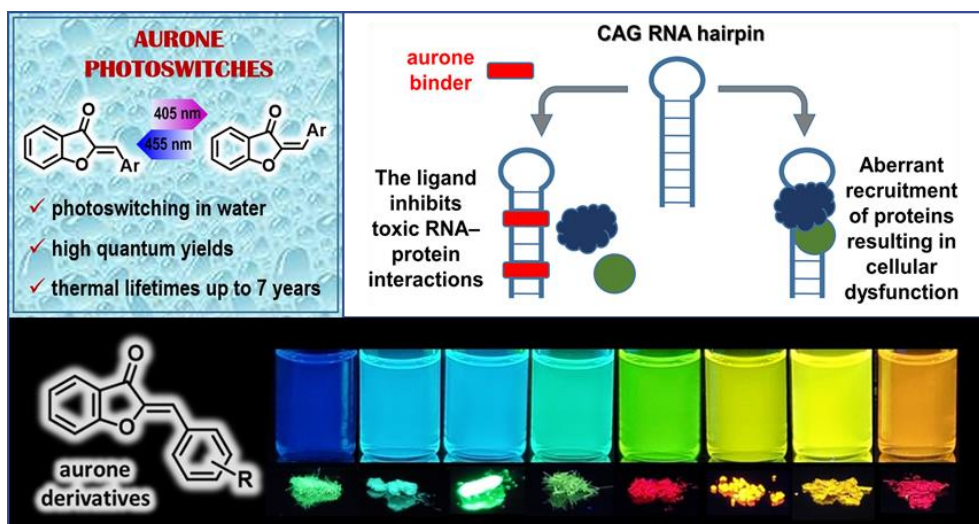
Aurones: from photoswitches to RNA binders and solid-state emitters

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Aurones are flavonoids derived from the 2-benzylidenebenzofuran-3(2*H*)-one scaffold. Pronounced biological activities of these molecules led to their extensive studies as drug candidates, while other properties did not gain enough attention. The aim of our work is to explore new possibilities in aurone chemistry. Thus, we introduced aurones as a novel class of visible-light photoswitches operating *in aqueous media* and possessing a highly advantageous combination of properties, as well as one of the longest half-lives of metastable forms in water (7 years) reported so far.[1] Further, we designed the first example of an aurone-based RNA binder targeting mutant RNA CAG repeat expansions in the Huntington's disease model.[2] Finally, we disclosed previously unknown solid-state fluorescence of aurones and formulated design principles for the dual-state emissive (DSE) aurone fluorophores.[3]



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Molecular-Level Insights into the Catalytic Activity of Hexafluoroisopropanol probed by Gas-Phase IR Spectroscopy

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Hexafluoroisopropanol (HFIP) has become an increasingly important solvent in organic chemistry due to its ability to accelerate reactions and improve their selectivity. These properties are attributed to HFIP's strong hydrogen-bond donor ability and the formation of small, long-lived aggregates with cooperatively strengthened terminal donor sites that can activate dissolved reactants.[1,2] Yet, molecular-level experimental insights into the specific interactions between HFIP and reactants remain scarce.

Here, we combine gas-phase infrared photodissociation (IRPD) spectroscopy, mass spectrometry, and electronic-structure calculations to obtain molecular-level insight into an HFIP-mediated reaction, using the hydrolysis of the kinetically stable hexafluorophosphate anion (PF_6^-) as a model system. Size- and composition-selected $\text{PF}_6^-(\text{HFIP})_m(\text{H}_2\text{O})_n$ complexes reveal that H_2O fundamentally alters the microsolvation behavior of HFIP. Rather than occupying the first solvation shell of PF_6^- , HFIP preferentially binds in the second shell, where the formation of an intersolvent hydrogen bond with H_2O cooperatively strengthens the $\text{H}_2\text{O}-\text{PF}_6^-$ interaction and may thereby facilitate the initial hydrolysis step.

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STM study of the Nucleation of Tris(dimethylamido)antimony on CoO Nanoislands

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In the search for an earth-abundant, eco-friendly and long-lasting alternative semiconductor material, mixed antimony chalcogenides (Sb_2E_3 , $\text{E} = \text{S}, \text{Se}$) have recently been investigated as they offer tunable bandgap with favorable optical and electrical properties^[1]. Building on previous reports of successful Sb_2S_3 and Sb_2Se_3 growth via atomic layer deposition (ALD)^[2], we focused on the first ALD half-cycle in greater detail. Therefore, we investigated the nucleation behavior of tris(dimethylamino)antimony on CoO nanoislands on Au(111) deposited by physical vapor deposition under ultrahigh vacuum conditions. We deposited tris(dimethylamino)antimony at varying temperatures and analyzed the prepared surfaces by scanning tunneling microscopy. Based on the previous studies^[3], we believe that, upon interaction with metal oxide surface, tris(dimethylamino)antimony loses all of its ligands, as we only observe antimony ions bound to surface atoms. The adsorption behavior of the ligands, however, remains unclear and requires further investigation.

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Probing fluorescence lifetimes of quantum dots in the gas phase

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Characterizing nanomaterials in the gas phase enables the investigation of intrinsic properties in the absence of interactions in an ensemble or with supporting media. This is enabled with a cryogenically cooled ion trap for single nanoparticle mass spectrometry [1], absorption spectroscopy [2], and fluorescence thermometry [3].

Here, we confine charged CdSe/CdS core/shell quantum dots (QDs) in the trap, and employ time-correlated single-photon counting to measure their fluorescence lifetimes. The dependence on shell thickness and trap temperature is investigated. Notably, the observed lifetimes are substantially shorter than values typically reported for comparable QDs in condensed-phase experiments [4]. The influence of the investigated parameters, as well as possible radiative and non-radiative decay channels contributing to the shortened lifetimes, are discussed.

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Molybdenum octahedral clusters and Vanadium polyoxometalates as photoinitiators and cross-linkers for functional PEGDA hydrogels with antibacterial properties

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Photopolymerization is a key methodology for synthesizing polymers and functional materials, as it enables precise spatial and temporal control over material formation, driven by chromophores that absorb ultraviolet or visible light to promote chain growth under irradiation.¹

{V₆O₁₉}-POMs and {Mo₆I₈}-clusters have emerged as promising candidates for next-generation photoinitiating systems distinguished by their unique electronic architectures.

The kinetics of photopolymerization was monitored by operando FTIR measurements. EPR spectra confirms propagating carbon-centered radicals.

Organo-functionalized metal (oxo)clusters simultaneously initiate free-radical photopolymerization and incorporate covalently into PEGDA networks through their terminal acrylate ligands. Scanning electron microscopy reveals dramatically different hydrogel morphologies. Functional hydrogels {Mo₆X₈}@PEGDA forms folded, three-dimensional "brain-like" structures due to its six-fold vinyl functionality. In contrast, {V₆O₁₉}@PEGDA produces smooth, flat films due to its limited two-terminal vinyl groups. {Mo₆X₈}@PEGDA hydrogels exhibits potent antibiotic-independent antibacterial activity against *E. coli*. The current work established a platform for integrating metal (oxo)clusters into polymer matrices with tunable morphology and antibacterial function.

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All-Photonic Yellow-Red-Blue-Green Orthogonal Photoswitching for Rewritable Four-Color 2D and 3D Displays and Optical Memories

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Photoswitches offer dynamic control over molecular states, often accompanied by distinct color changes arising from their absorption profiles. While numerous photoswitches exhibit reversible switching between colorless and colored states, combining two photoswitches can, in principle, generate four distinct states and associated colors using light irradiation.^[1] However, only limited systems have demonstrated such multicolor switching, often relying on potentially harmful UV light. Moreover, achieving primary colors through coupled photoswitches requires careful selection of switches with appropriately separated absorption profiles. In this work, we report^[2] a minimal photoswitching strategy enabling alteration between four distinct colors, yellow, red, blue, and green in response to NIR and visible light irradiation. The resulting four states can be interconverted in a fully orthogonal and reversible manner, which was integrated into a solid matrix, enabling the fabrication of unique two- and three-dimensional displays based on four-color combinations performing versatile platform for multistate optical information display and photonic applications.

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Engineering the Implant–Bone Interface: Mesoporous Bioactive Glass Nanoparticle-Enriched Coatings on β -Titanium Alloys

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β -Titanium alloys are promising implant materials due to their non-toxic composition, low elastic modulus, high biocompatibility, and good corrosion resistance [1]. The implant–bone interface plays a crucial role in osseointegration. This study aimed to develop chitosan coatings containing antibacterial silver nanoparticles and magnesium-modified mesoporous bioactive glass nanoparticles (MBGN-Mg) on Ti13Nb13Zr alloy and evaluate their physicochemical and biological properties. Uniform and stable coatings were obtained. Incorporation of MBGN-Mg increased surface roughness, wettability, and surface free energy compared with plain chitosan/Ag coatings, which may promote protein adsorption and cell adhesion [2]. MBGN-modified coatings also exhibited improved adhesion to the substrate, maintaining their integrity after tape testing, unlike the control coatings. Electrochemical analysis in simulated body fluid revealed acceptable corrosion behavior. MBGN-enriched coatings provide a multifunctional interface with enhanced surface topography and bioactivity while preserving the corrosion resistance of Ti13Nb13Zr, demonstrating their potential for orthopedic implant applications. Further studies will focus on evaluating the cytocompatibility of the developed coating systems and adapting this surface modification strategy to other β -titanium alloy, Ti35Nb7Zr5Ta.

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Poster Abstracts

Synthesis of Asymmetric Cyclophanes for the Recognition of Nucleotides

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Cyclophanes are a type of macrocycle that have been developed and studied for nucleotide detection in recent years.¹ Their chemical structures can be modified to enhance their interactions with nucleotides and the resulting response.² The synthesis of these asymmetric macrocycles was centered on a naphthalimide fragment connected to a nitrogen-containing heterocyclic ring through azaethyldiamine chains, to obtain properties such as water solubility and a measurable fluorescence response upon nucleotide interaction (Figure 1). Their interactions with nucleotides were investigated through aggregation UV-Vis experiments, pH-dependent fluorescence scans, and fluorescence titrations. The results showed different fluorescence responses depending on the nucleotide. Pyridine-based macrocycles exhibited a selective fluorescence increase upon interaction with ATP, whereas the pyridinium-based cyclophane showed fluorescence quenching to different degrees. These findings demonstrate the potential of cyclophanes as fluorescent probes for selective nucleotide recognition and detection.

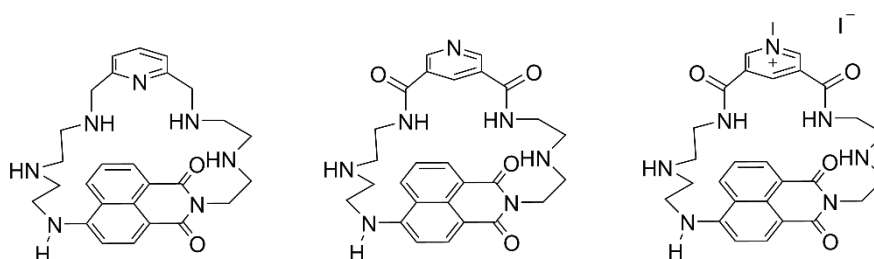


Figure 1. Structures of the synthesized asymmetric cyclophanes as nucleotide receptors.

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Comparison of various L-arginine functionalized Au-Fe₃O₄ nanostructures in Cancer Radiation Therapy

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Currently, surgery, chemotherapy and radiotherapy are widely used in clinics for breast cancer treatment. However, some tumors may not be discovered in time for surgical intervention and non-surgical methods are often limited by severe side effects. In addition, heterogeneity of tumor tissues as well as resistance of cancer cells towards monotherapies indicates the necessity to combine two or more modalities of cancer treatments. Fe₃O₄ nanoparticles (NPs) are good candidates as radiosensitizers in radiation therapy by generating high level of hydroxyl radicals via the Fenton reaction. Unfortunately, Fe₃O₄ nanoparticles gradually oxidize to Fe₂O₃ under ambient conditions losing their ability to catalyze the Fenton reaction. In recent publications Au-Fe₃O₄ nanoheterodimers, Au-Fe₃O₄ nanoflowers and patchy Fe₃O₄@Au NPs were developed as excellent Fenton catalyst, that are stable against oxidation. These nanoparticles were functionalized with the NO donor L-arginine, which ensured their water solubility and biocompatibility. In irradiated breast cancer cells MCF-7, all NPs generated the highly toxic hydroxyl radical via Fenton reaction and peroxynitrite, which arise from the reaction of NO with superoxide. In irradiated 3D multicellular tumor spheroids (MCTS), NHDs were the most efficient radiosensitizers by causing an enormous shrinkage of the MCTS. However, multicellular spheroids (MCS) of non-tumorigenic MCF-10A cells treated with NHDs also decreased in volume. In contrast, patchy Fe₃O₄@Au NPs significantly diminished the MCTS volume upon X-ray radiation, but have no influence on the MCF-10A MCS volume.

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Environmental cues shape the biogenesis and function of extracellular vesicles in *Streptococcus pneumoniae*

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Streptococcus pneumoniae adapts its metabolism during host invasion and releases extracellular vesicles (Sp-EVs), although the relationship between metabolic adaptation and vesicle biogenesis remains unclear. We investigated how environmental cues affect Sp-EV production and function. Pneumococci were exposed to normal human serum (NHS) and grown under different temperature, pH, and glucose conditions. Super-Resolution Structured Illumination Microscopy was performed to study bacterial exposure to NHS. Sp-EVs were characterized by nanoparticle tracking analysis, while their function was investigated by a multi-omics approach and biofilm assays. NHS induced cell wall rearrangement and markedly increased Sp-EV production. Moderate glucose availability and incubation at 37°C also enhanced vesicle yield. Proteomic analysis revealed enrichment of carbon metabolism-related proteins in Sp-EV cargo, with GlmU, SpuA, BgaA, and IlvC upregulated in glucose-associated Sp-EVs. Vesicular DNA carried mutations in genes linked to competence and sugar transport. Functionally, Sp-EVs promoted biofilm formation in both *S. pneumoniae* and *Streptococcus pyogenes*. These findings demonstrate that environmental conditions shape Sp-EV biogenesis and cargo, providing insight into the strategies employed by *S. pneumoniae* during infection.

Cofacial Nanographene Dimers

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Nanographenes are large polycyclic aromatic hydrocarbons (PAHs) that exhibit outstanding absorption and luminescence properties. For instance, hexa-*peri*-hexabenzocoronene (HBC) based nanographenes have been extensively investigated over the last decades tailoring their unique electronical and photo-physical properties.^[1] In contrast, research into cofacial PAH dimers has gained increasing interest due to the observation of mixed excited-states, which can lead to excimer formation and singlet fission.^[2] Herein, we show the synthesis of HBCs which are rigidly connected to a xanthene unit to form H-type dimers. Different HBC-dimers have been synthesized by the insertion of phenyl spacers modifying the overlap between both chromophores (**Figure 1**). The differently shifted HBC units can be analyzed with respect to their molecular orbital interactions, potentially revealing mixed excited-state interactions.

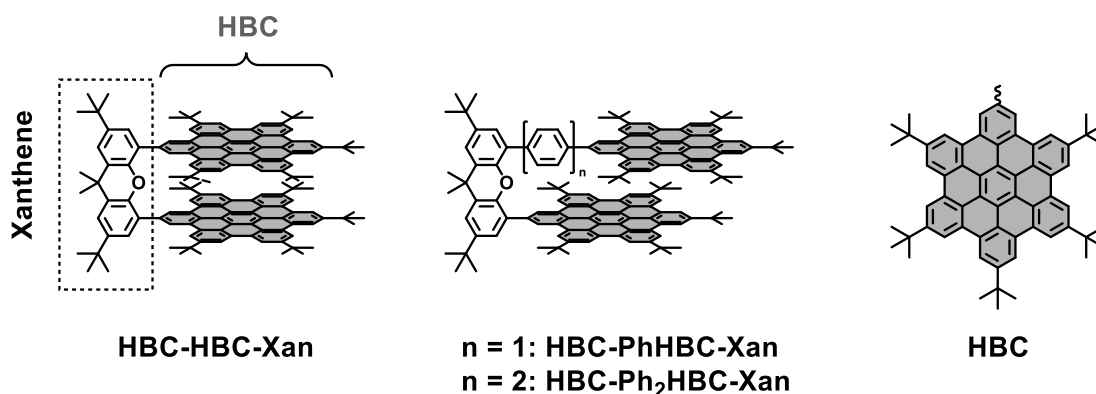


Figure 1. Overview of xanthene bridged HBC bilayer systems.

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Molecular-Level Insights into the Catalytic Activity of Hexafluoroisopropanol probed by Gas-Phase IR Spectroscopy

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Hexafluoroisopropanol (HFIP) has become an increasingly important solvent in organic chemistry due to its ability to accelerate reactions and improve their selectivity. These properties are attributed to HFIP's strong hydrogen-bond donor ability and the formation of small, long-lived aggregates with cooperatively strengthened terminal donor sites that can activate dissolved reactants.[1,2] Yet, molecular-level experimental insights into the specific interactions between HFIP and reactants remain scarce.

Here, we combine gas-phase infrared photodissociation (IRPD) spectroscopy, mass spectrometry, and electronic-structure calculations to obtain molecular-level insight into an HFIP-mediated reaction, using the hydrolysis of the kinetically stable hexafluorophosphate anion (PF_6^-) as a model system. Size- and composition-selected $\text{PF}_6^-(\text{HFIP})_m(\text{H}_2\text{O})_n$ complexes reveal that H_2O fundamentally alters the microsolvation behavior of HFIP. Rather than occupying the first solvation shell of PF_6^- , HFIP preferentially binds in the second shell, where the formation of an intersolvent hydrogen bond with H_2O cooperatively strengthens the $\text{H}_2\text{O}-\text{PF}_6^-$ interaction and may thereby facilitate the initial hydrolysis step.

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Towards Accurate Core-Level Spectroscopy: Connecting Δ SCF Core-Hole Localisation with GW

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Accurate theoretical core-level binding energies are essential for interpreting X-ray photoelectron spectroscopy, but remain challenging because core ionisation induces strong electronic relaxation and screening. The GW approximation provides a many-body framework for electron-removal energies and has achieved high accuracy for molecular core levels. Here, we investigate complementary Δ SCF calculations for carbon 1s ionisation, focusing on the reliable construction and identification of atom-specific core-hole states. PBE and PBE0 calculations are combined with constrained Δ SCF, analysis of Kohn-Sham orbital coefficients, spin-density distributions, and Boys localisation. Molecular systems with chemically inequivalent and symmetry-related carbon atoms are used to examine when canonical core orbitals can be assigned directly to individual atomic sites and when orbital mixing complicates this assignment. Establishing robust atom-resolved core-hole states provides a reference for analysing relaxation effects and supports systematic comparison with GW core-level binding energies.

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From Plate to Pee: First Evidence for the Bioavailability of Dietary Kukoamines

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Kukoamine A and B are bioactive phenolic polyamine alkaloids naturally occurring in Solanaceous plants, including potatoes. Dietary kukoamines are of interest because both isomers act as μ -opioid receptor agonists and may mediate physiological effects such as gastrointestinal modulation, reward processes, and analgesia. [1] However, their bioavailability, metabolism, and excretion in humans remain largely unknown.

This case study gained first insights into the bioavailability of potato-derived kukoamines by monitoring their urinary excretion over 24 h.

Using LC-MS/MS, free kukoamine concentrations were determined in the urine over time. Additionally, urine samples were analyzed for the presence of glucuronide and sulfate conjugates of kukoamines using enzymatic hydrolysis. While no kukoamine phase-II metabolites were detected in urine, urinary excretion of kukoamine A and B peaked at roughly 5 hours, with kukoamine B excretion of up to 7 ng/g creatinine.

These findings provide initial evidence for the systemic availability of potato-derived kukoamines and lay the foundation for a larger human pilot study.

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The Confusion is Real: GRAPHIC – A Network Science Approach to Confusion Matrices in Deep Learning

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Artificial intelligence systems that sort images into categories make mistakes, and these mistakes are rarely random. A network confuses a leopard with a tiger far more often than with a bicycle. Which classes get mixed up tells us how a machine sees the world, yet is rarely examined. We present GRAPHIC [1], an architecture-agnostic method that analyzes neural networks class by class. Using linear classifiers, we read a confusion matrix out of every layer, a table counting how often one class is taken for another, and treat it as a network whose nodes are classes and whose links are confusions. Network science then quantifies how these networks reorganize across layers and training epochs, revealing which classes are linearly separable, how architectures behave, and where datasets are flawed. GRAPHIC flagged ambiguous images that participants in a human study confused in the same way as the machine.

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Selective multistate switching enabled by intramolecular H-bond in a hemithioindigo switch

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Molecular switches convert between distinct states in response to external stimuli, most commonly light, heat, or pH. Here, we present a novel switch based on Hemithioindigo (HTI) scaffold that can be selectively addressed into any of three states, each accessed via a different stimulus. HTI-based photoswitches are well-known for their photo- and thermostability and for high enrichment levels attainable in each state [1]. By introducing a fixed sulfoxide stereocenter into the HTI core, we further enable the design of molecular motors and observe modes of molecular motion beyond those typical of the overcrowded alkene-motor cycle.

Building on a system studied in our group [2], we introduced a phenolic moiety into the scaffold, which stabilizes the structure through intramolecular hydrogen bonding and thereby confers selectivity to the thermal step of the switching cycle. The acidity of the Ph-OH group further opens access to additional, otherwise inaccessible transformations available only in the anionic state.

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Text analysis Workflow for non-structured Laboratory Documents

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Laboratory documents often contain relevant administrative and scientific information in heterogeneous PDF formats, including digitally generated files, scanned pages, tables, and stamped regions. Reviewing such documents manually can be time consuming, repetitive, and prone to inconsistencies. This highlights the need for automated workflows supporting standardized and efficient document analysis [1] [2]. This work presents an approach for automated key information extraction through the analysis of documents with laboratory analysis related data. It combines document text extraction with targeted optical character recognition (OCR) for scanned or visually embedded content such as logos or stamps. The workflow was developed to support structured document screening and to improve the accessibility of relevant data such as sender, receiver, data of arrival and order information, for subsequent analyses. Rule-based text processing and keyword detection are applied to identify relevant document sections and classify extracted information into predefined categories. Further development will focus on improving layout understanding of varying document formats and reducing false-positive detection types while maintaining data protection and confidentiality requirements.

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Surface Hopping Dynamics with MRSF-TDDFT: Interfacing OpenQP and SHARC

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Mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT) is a novel electronic-structure method that is well suited for nonadiabatic molecular dynamics simulations due to its TDDFT-like computational cost and notable advantages over linear-response TDDFT, including the description of (some) double excitations and the correct topology at conical intersections. The inclusion of spin-orbit couplings has recently extended its potential applications to systems involving intersystem crossing processes.

Inspired by our recent study on photocyclization mechanisms in aza-Diarylethenes,^[1] where we performed nonadiabatic dynamics using MRSF-TDDFT, we present a new flexible interface that enables surface-hopping simulations at the MRSF-TDDFT level within the SHARC^[2] framework, using OpenQP^[3] as the electronic-structure engine. Low-level access to OpenQP allows for tailored calls according to the required features and efficient reuse of cached data at each time step. The seamless integration with SHARC enables convenient trajectory setup, execution, and analysis within a single framework. Furthermore, QM/MM hybrid simulations are now possible through SHARC's QM/MM interface, combining OpenQP for the QM region with OpenMM for the MM region.

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Visible-Light-Driven Self-Catalyzed 6 π -Electrocyclization to Chromenopyrazolines

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Photocatalysis is a transformative tool in synthetic chemistry. However, its sustainability is limited due to the reliance on non-abundant and expensive transition metal-based and waste-generating organic dyes as photocatalysts. Efficient approaches eliminating the need for a photocatalyst, by relying only on the photoactive nature of the substrate, are highly attractive, yet remain rare. We report the first self-catalyzed, visible-light induced electrocyclization reaction that enables direct access to new chromenopyrazolines from readily available acyl hydrazones, without the need for external photocatalysts or additives. This photo-autocatalytic strategy exploits the substrates' intrinsic photoactivity, i.e. light initiated E/Z-isomerization and change in NH acidity, to drive electrocyclization, obviating external photocatalysts and minimizing waste. The reaction proceeds under very mild conditions to deliver chromenopyrazolines in up to 96% yield. By uniting operational simplicity, atom economy, and environmental compatibility, this work establishes a green and broadly applicable platform for constructing chromenopyrazoline frameworks of relevance to life science.^[1]

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Porphyrin-Fused Helical Multilayer Nanographenes

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Helical nanographenes have gained considerable attention due to their non-planar π -conjugated structures and chiroptical properties. Increasing the size of the π -system and introducing multilayer arrangements can significantly affect their electronic and photophysical properties.^[1,2]

In this work, porphyrins are incorporated into helical multilayer nanographene systems. Ethynyl-functionalized phenanthrene building blocks are used to form extended aromatic structures by Diels–Alder reactions and oxidative cyclodehydrogenation. Oxidative β -meso five-membered ring fusion is subsequently used to connect the porphyrin units directly to the nanographene π -system.^[3,4]

The synthesized compounds will be characterized to study the influence of porphyrin fusion on the structural, optical and electronic properties of the helical π -systems.

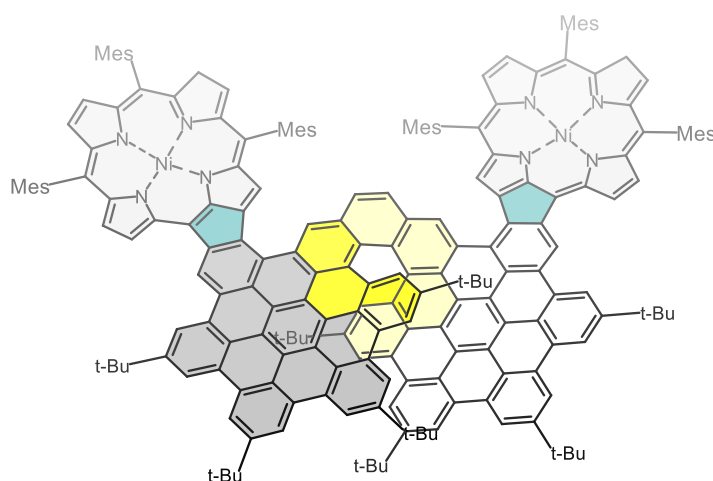


Figure 1. example of π -extended porphyrin-containing helical nanographene system.

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CHIRAL N-ATOM DOPED NANOGRAPHENES

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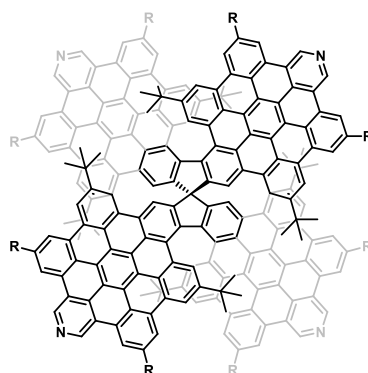
Chiral nanographenes combine the unique properties of inherently chiral molecules with the optical, electronic and magnetic properties of nanographenes. [1] This fascinating class of polycyclic aromatic hydrocarbon structures can find new applications in the field of nanoelectronics, optoelectronics and spintronics. [2]

Another strategy to modulate the properties of graphene is doping with heteroatoms, which can induce exotic features such as ferromagnetism but most importantly it can enhance the conductivity of the material and promote the formation of a band gap. [3,4]

By combining chirality and doping, a new set of optoelectronic and photophysical properties can be generated, opening a new field of potential applications in nanoelectronics. [2,3]

In this work, so called pyridinic nanographenes are linked with the inherently chiral molecule spirobifluorene by different cross-coupling reactions and subsequent Scholl oxidation.

The synthesized compounds will be characterized to study the influence of contortion and doping on the structural, optical and electronic properties of presented systems.



R = H/Bu

Figure 1: Example of Chiral Pyridinic Nanographene.

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Heterogeneously Catalyzed Energy Release of Azaborine based Molecular Solar Thermal Systems

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Molecular solar thermal (MOST) systems enable solar energy conversion, storage, and release using switchable photoisomers.[1] Azaborine/BN-Dewar couples are promising MOST candidates, but energy release has so far relied on homogeneous catalysts, complicating catalyst–photoisomer separation.[2,3] Here, we investigate heterogeneous energy release from three azaborine/BN-Dewar systems (Aza1/Dew1, Aza2/Dew2, Aza3/Dew3) on Au(111). We tested cyclohexane and dichloromethane as solvents and used highly oriented pyrolytic graphite as an inert reference surface. We combined photochemical infrared reflection absorption spectroscopy (PC-IRRAS) with density functional theory (DFT). We show that Au(111) catalyzes BN-Dewar back-conversion and releases the stored energy, with activity strongly depending on substituent and solvent. Although Au(111) is insufficiently active for practical implementation, our results demonstrate that heterogeneous catalysis can trigger energy release in azaborine/BN-Dewar MOST systems.

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Solution-processed In₂S₃ nanoparticles for thin-film photovoltaic application

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The highest-efficiency devices using Sb₂S₃, a promising thin-film solar absorber due to its stability, non-toxicity, and strong absorption in the visible, rely on cadmium-based electron transport layers. Herein, we focus on In₂S₃ NPs as a stable and non-hazardous electron-conducting alternative. We synthesized crystalline, stoichiometric β -In₂S₃ by a wet-chemical route, shifting the band gap toward the UV/blue region through quantum confinement, thereby minimizing spectral overlap with Sb₂S₃. Purification and processability were optimized by a liquid-phase ligand exchange procedure, enabling film formation below 100 nm thickness. Their optoelectronic application was verified in PV devices, investigating the effect of post-processing treatments (thermal or solid-phase ligand exchange treatments) toward band-level alignment for electron extraction and film conductivity.

This PV framework serves as a photoelectrode model, in which NiO NPs serve as the hole-selective contact and catalyst for alternative anodic oxidation reactions other than water oxidation. The electrocatalytic performance was confirmed previously toward the oxidation of 5-hydroxymethylfurfural, relevant to biobased chemical feedstock production. With this, we aim to directly convert solar energy to chemical energy.

Targeting Makes the Difference: Single-Cell Imaging Reveals Enhanced Mitochondrial Superoxide Scavenging by a Novel Mitochondria-Targeted MnSOD Mimetic

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Reactive oxygen species (ROS), particularly mitochondrial superoxide, contribute to oxidative damage and are implicated in aging and diseases. Therapeutic potential of superoxide dismutase (SOD) mimetics is often limited by insufficient mitochondrial accumulation.

Here, we present a novel mitochondria-targeted MnSOD mimetic obtained by conjugating the established Mn pentaaza macrocyclic complex Mn-Pyane with a triphenyl phosphonium (TPP⁺) moiety to promote mitochondrial delivery. The compound was evaluated in MCF10A ("healthy" breast cells), MCF7 (breast adenocarcinoma cells) and SH-SY5Y (neuroblastoma cells). Cellular uptake and distribution were quantified by ICP-MS, while cytotoxicity, mitochondrial membrane potential, and oxidative stress were assessed using established assays. Total intracellular ROS were determined using dihydroethidium (DHE), whereas mitochondrial superoxide was quantified by confocal microscopy using MitoSOX and an automated CellProfiler-based analysis.

The targeted MnSOD mimetic showed enhanced mitochondrial accumulation, more efficient scavenging of mitochondrial superoxide, reduced off-target effects, and improved long-term cell viability, demonstrating the advantages of mitochondrial targeting over Mn-Pyane.

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Enhancement of Photoconductivity upon Complexing Perylene Bisimide Cyclophane - Fullerene Hybrid with [10]CPP

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Perylene bisimide (PBI) cyclophanes are attractive photoactive platforms because their cofacial chromophores promote strong excitonic interactions and symmetry-breaking charge transfer. However, translating these molecular excited-state processes into efficient charge transport and photocurrent generation remains challenging. Herein, we investigate how fullerene functionalization and supramolecular encapsulation influence the photophysical and electrochemical properties of the PBI cyclophane **P2**. We compare **P2** with the fullerene-containing derivative **P2(C₆₀)₂**, the covalently-functionalized fullerene analogue **P2F2C₁₈**, and the bis-pseudorotaxane **([10]CPP)₂→P2(C₆₀)₂** obtained by complexing both C₆₀ termini with [10]cycloparaphenylene ([10]CPP). The cofacial PBI arrangement governs the excited-state behaviour of the series, producing H-type excitonic coupling, fluorescence quenching, charge-transfer, and non-radiative relaxation pathways. All systems exhibit stable photoactivity and n-type semiconductor behaviour. Incorporation of electronically accessible C₆₀s substantially increases the photocurrent and -potential in **P2(C₆₀)₂** relative to **P2**. Remarkably, **[10]CPP** encapsulation of **P2(C₆₀)₂** enhances conductivity and photoresponse, without compromising photostability or the intrinsic photophysical properties of the PBI core. These findings identify fullerene accessibility and supramolecular organization as key parameters connecting molecular excited-state dynamics with macroscopic photoelectrochemical performance, establishing nanohoop encapsulation as a promising non-covalent strategy for optimizing organic photoactive materials.

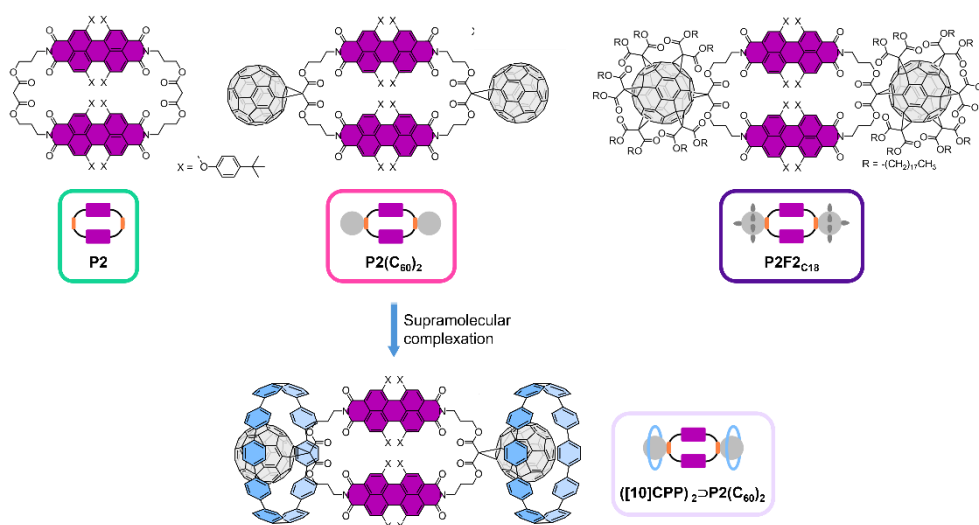


Fig 1. PBI-based molecular structures analyzed in this work.

From Underpotential to Multilayer Growth: A Potential- and Time-Resolved AFM Study of Selenium Deposition in Electrochemical ALD

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Electrochemical atomic layer deposition (EC-ALD) enables atomic-level control of semiconductor thin films like In₂Se₃ via solution processing [1]. Self-limiting growth, essential for ALD, is achieved through underpotential deposition (UPD), where a monolayer of Se deposits at potentials more positive than thermodynamic deposition.

This work explores potential- and time-dependent Se deposition on Au(111) using in situ electrochemical atomic force microscopy (EC-AFM) and cyclic voltammetry (CV), across three regimes: (1) UPD (between +0.45 V_{RHE} and +0.60 V_{RHE}) yielding slow, self-limiting submonolayer growth with preserved substrate morphology; (2) mixed UPD/bulk deposition (between +0.10 V_{RHE} and +0.45 V_{RHE}), causing rapid island formation and non-uniform films; (3) bulk deposition (below +0.10 V_{RHE}) leading to slower multilayer growth with island formation. Notably, the Au(111) surface structure remains intact even after prolonged deposition. These results underscore the importance of precise potential and time control in EC-ALD to minimize defects and achieve high-quality films.

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Towards structure-informed aptamer design: investigating interactions of RNA aptamers with GntR/HutC bacterial repressors

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Bacterial repressors are widely used for controlled gene expression, for example, in synthetic biology. Synthetic RNA aptamers can be used to regulate these proteins' activity by blocking DNA-binding domain as an alternative to native effectors – small molecules that regulate repressors allosterically. Here, we present the crystal structures of transcriptional factors DasR (from *Streptomyces coelicolor*) with aptamer Dap1 (PDB: 9I0V, [1]) and NagR (from *Bacillus subtilis*) with aptamer Nap1. We investigated the individual contributions of amino acids from the interaction interfaces to complex formation and found that sequence specific contacts involved in binding RNA aptamers replicate interactions involved in complex formation with DNA that are native for the repressors [2]. The similarities of the folds of the aptamers that were derived independently suggest the possibility to use them as blueprints for rational design of RNA aptamers targeting other bacterial transcriptional factors.

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Carbonate Looping Clusters for the Carbon Capture from biomass combustion plants

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The CarbonateClusters project focuses on Bioenergy Carbon Capture and Storage (BECCS) as a strategy for implementing land-based Carbon Dioxide Removal (CDR) to enable Negative Emissions. The proposed approach uses a novel open Carbonate Looping Processes that involves decentralized capture of biogenic CO₂ in small-scale biomass combustion plants and the release of this CO₂ in larger-scale calcination plants. An electrically heated steam calciner provides CaO sorbent with ideal proper-ties for the carbon capture at decentralized small- and medium scale bioenergy sites and provides biogenic carbon for geological sequestration. Key innovations are the electrically heated steam calciner and a new CO₂ adsorber concept based on hot gas precoat filtration. A socio-economic assessment will compare economic impacts and will analyze funding policies that might favor “green” carbon cred-its and negative emission technologies and the technology’s contribution to the United Nations Sus-tainable Development Goals (SDGs). The CarbonateClusters concept therefore effectively contributes to the federal government’s climate neutrality targets by enabling negative CO₂ emissions.

Size Estimation Of Optically Trapped Nanorods

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Levitated nanoparticles serve as a platform for studying quantum mechanics in macroscopic systems [1]. Most of the levitation experiments use spherical particles. However, recent studies of librational and rotational motions of trapped particles naturally rely on particles of anisotropic, i.e., elongated shape [2]. In any related experiment, the knowledge about the size or mass of the levitated particle is essential. Here, we present a method to determine the size of a levitated nanorod. The nanorod is modeled as a capsule-shaped particle having a cylindrical part with two hemispherical end caps. From the damping of the translational motion of such a rod, we induce its length and diameter. Using optically levitated silica nanorods, we show that with this method we can distinguish a cluster from a single particle and infer the size of single trapped nanorods. Our method can be applied in a broad range of experiments on levitodynamics with rod-shaped particles.

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Hexabenzocoronene–Benzimidazole Hybrid Architectures and Faraday Rotation of the First Hexabenzocoronene–Phthalocyanine

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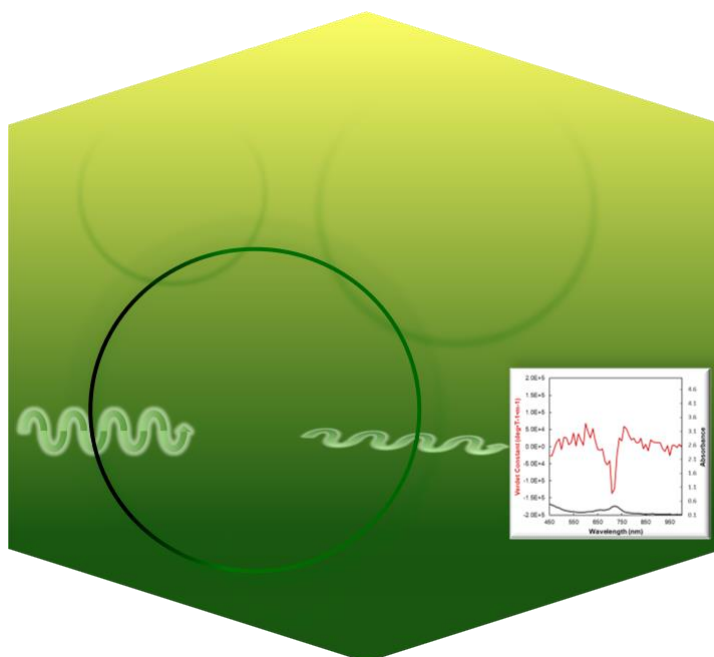
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The synthesis and characterization of a first example of a Ni-phthalocyanine (Pc) hybrid molecule carrying four hexa-peri-hexabenzocoronene (HBC) substituents and of three HBC-benzimidazole derivatives is reported. These π -electron rich chromophores exhibit a high molar absorption coefficient with extended absorption up to 460 nm. Particularly, HBC-Pc absorbs throughout most of the UV–vis range with the Pc Q-band located at 672 nm. This enables its investigation as a Faraday rotator where it displayed a remarkable Verdet constant of $-1.4 \times 10^5 \text{ deg T}^{-1}\text{m}^{-1}$ at 700 nm assigned to Faraday A-term activity. Electrochemical measurements supported by DFT calculations elucidated the electronic structure of the molecules together with excited state molecular orbital analysis using TDDFT. Here, HBC-Pc showed a HOMO/LUMO gap considerably lower than the other HBC-based compounds due to the introduction of the Pc scaffold.



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All-Photonic Yellow-Red-Blue-Green Orthogonal Photoswitching for Rewritable Four-Color 2D and 3D Displays and Optical Memories

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Photoswitches offer dynamic control over molecular states, often accompanied by distinct color changes arising from their absorption profiles. While numerous photoswitches exhibit reversible switching between colorless and colored states, combining two photoswitches can, in principle, generate four distinct states and associated colors using light irradiation.^[1] However, only limited systems have demonstrated such multicolor switching, often relying on potentially harmful UV light. Moreover, achieving primary colors through coupled photoswitches requires careful selection of switches with appropriately separated absorption profiles. In this work, we report^[2] a minimal photoswitching strategy enabling alteration between four distinct colors, yellow, red, blue, and green in response to NIR and visible light irradiation. The resulting four states can be interconverted in a fully orthogonal and reversible manner, which was integrated into a solid matrix, enabling the fabrication of unique two- and three-dimensional displays based on four-color combinations performing versatile platform for multistate optical information display and photonic applications.

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MPS for the Observation of Subtle Changes in Iron Oxide Phases and Its Application to Hydrogen Detection

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Magnetic particle imaging and magnetic particle spectroscopy (MPS) have primarily been developed for biomedical applications, including imaging and tracer characterization.^[1] Beyond these applications, the sensitivity of MPS to the magnetic properties and interactions of nanoparticles offers the possibility of monitoring subtle transformations within particle-based systems. Here, we demonstrate this capability using a model system responsive to hydrogen exposure. Iron oxide-based supraparticles containing platinum nanoparticles were exposed to hydrogen, inducing chemical transformations of the iron oxide phase. The resulting changes in magnetic response were investigated by MPS. MPS sensitively resolves changes associated with hydrogen-induced reduction of the iron oxide phase. Owing to its fast, simple, and non-destructive nature, MPS enables the influence of parameters such as hydrogen exposure time and gas composition on the reaction to be monitored. Thus, MPS provides a valuable complementary technique to established methods such as SQUID magnetometry and Mössbauer spectroscopy for investigating iron oxide transformations. These findings provide a basis for future magnetic hydrogen-sensing applications.

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Automated Bacterial shape Recognition in Microscopy Images using deep learning

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Rapid identification of bacteria from microscopy images is essential for clinical diagnostics, quality control and environmental monitoring. However, it remains challenging, since manual assessment can be time-consuming and subject to differences in interpretation. This work develops a computer vision pipeline that detects and classifies bacterial cells. A bacterial slide image dataset was annotated using CVAT, with bounding boxes and shape labels assigned to the corresponding morphological classes[1]. Two detection architectures were trained and compared; YOLO, a single stage real time detector and a two-stage detector Faster R-CNN with a ResNet-50 FPN backbone. To ensure a fair comparison, both models were trained under identical settings such as data split, input resolution and number of epochs. Performance was assessed using mean average precision, per-class precision, recall and F1 score. The results demonstrate that shape based automated detection provides a reliable and scalable route to bacterial identification[2]. Future work is extending the pipeline to incorporate color information from bacterial samples, enabling combined shape and gram-stain based classification for more detailed species level identification.

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Multimeric Norbornadiene/Quadricyclane Photoswitches as Potential Candidates for Molecular Solar Thermal Application

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A major challenge associated with the utilization of the sun as a sustainable energy source is the storage of solar energy [1]. A promising approach to tackle this problem is the use of molecular solar thermal (MOST) systems [2]. Upon irradiation with sunlight a stable parent compound A undergoes isomerization towards a meta-stable isomer B. If the system is converted back to compound A, the stored energy can be released in the form of heat. [3]

The Norbornadiene (NBD)/Quadricyclane (QC) interconversion couple is a well-researched candidate for MOST applications due to its potential for high energy storage density [4].

By attaching multiple NBD scaffolds to one linker, the gravimetric energy density of the system can be increased and the absorption properties of the NBD photoswitch enhanced [5]. We present a library of multimeric NBD derivatives featuring a central electron withdrawing unit. The photophysical properties of all compounds were investigated employing UV/Vis and NMR spectroscopy as the main characterization methods.

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C5a is a potent chemotactic factor for neutrophils and influences the expression of surface and activation markers

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Complement activation and neutrophil infiltration are key drivers of renal inflammation, particularly in ischaemia-reperfusion injury and acute kidney diseases. However, the interaction between neutrophils and complement remains unclear. This study investigated the effects of C5a on neutrophil migration, complement receptor expression, and activation markers.

Human neutrophils were isolated from blood samples and stimulated with C5a (0.1–100 nM) in a Transwell chemotaxis assay. Cells were subsequently incubated with the most effective C5a concentration and analysed by flow cytometry. Expression of complement receptors (C3aR1, C5aR1, C5aR2, CD11b, CD11c, CD35), CD66b, TLR4, and activation markers CD63 and CD69 was compared with LPS-stimulated and untreated controls.

C5a induced dose-dependent neutrophil migration, with maximal effects at 10 nM. This concentration increased C5aR2, CD11b, CD11c, CD66b, CD63, and CD69 expression, while significantly reducing surface C5aR1. C3aR1 and CD35 remained unchanged. C5a-induced activation was stronger than LPS stimulation.

These findings demonstrate that C5a is a potent neutrophil chemoattractant and activator, suggesting an important role in complement-mediated renal inflammation.

Characterization of B cells as drivers of early inflammatory arthritis in K/BxN mice

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Despite their diagnostic value, the role of autoreactive B cells and their autoantibodies in the pathogenesis of rheumatoid arthritis (RA) remains debated. To assess the influence of the B cell compartment and downstream effects during early inflammatory arthritis we used the K/BxN mouse model, which spontaneously develops an inflammatory joint disease highly similar to human RA. In this model the underlying break of tolerance is driven by a transgenic T-cell-receptor, while B cells and their autoantibodies have been shown to be essential for triggering the inflammation. We thus set out to analyse the role of the B cells in early disease onset to find new therapeutic approaches for human RA.

Analyzing the pre and early inflammatory phases of the model disease, we found a germinal center driven B cell response starting at the onset of joint inflammation. We could show that this response was localized to the joint draining lymph nodes and spleen. Additionally, B cell development in general appears to be dysregulated. While B cell activation can likely be attributed to increased interaction with Tfh cells, both activation and developmental dysregulation could also potentially be influenced directly by Th17 axis cytokines. In line with these findings we could for the first time show an increase in not only IgG1 autoantibodies but also an increase in IgE levels. This increase appears to be coupled to an increase in innate effector cell frequency and activation.

In summary, we could demonstrate that the B cells drive the disease by modulation of other innate immune cells via their Fcγ receptors and thus are key targets in RA therapy

Modulating Cytotoxic T Cell Responses via ATM or ATR Inhibition and Hypofractionated Radiotherapy in a 3D HNSCC Co-Culture Model

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HPV-negative head and neck squamous cell carcinoma (HNSCC) exhibits increased radioresistance. Inhibition of the DNA damage response (DDR) via ATM or ATR represents a promising strategy to overcome this resistance, though effects on tumor-immune interactions remain unclear.^[1,2] Here, we established 3D HNSCC spheroids, co-cultured with stimulated cytotoxic T cells, to investigate how tumor cells treated with ATM inhibitor AZD0156 or ATR inhibitor VE-822 ± hypofractionated irradiation (2×5 Gy) affect T cell function.^[3]

T cell activation, proliferation, migration and spatial infiltration into spheroids were assessed by flow cytometry, Transwell assays and imaging-based methods.

ATRi+RT-treated spheroids maintained or increased T cell activity, whereas ATMi±RT-treated spheroids consistently reduced it, suggesting ATMi, unlike ATRi, may rather act as an immunosuppressive effector of T cell function, pointing to distinct immunomodulatory effects that warrant further investigation.

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