Women in Science

3rd Erlangen Symposium

July 22-24, 2024

Book of Abstracts

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Foreword

As the members of the Women in Science-Erlangen Symposium Organizing Committee, it gives us immense pleasure to welcome you to the 3^{rd} edition of our symposium series at the Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg in Germany.

The Women in Science-3^{rd} Erlangen Symposium has been organized by female doctoral students, postdoctoral researchers, and a junior group leader from the Department of Chemistry and Pharmacy 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 providing inspiration for young scientists.

We are delighted to welcome more than 140 participants from many different career stages to the 3^{rd} edition of our symposium. Over the course of three days, top-notch female scientists from diverse research fields such as organic chemistry, computational chemistry, catalysis and materials science, 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 keynote and invited lectures, 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 during the round-table discussion. 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 individual 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.

Organizing Committee WIS24

Scientific Advisory Committee

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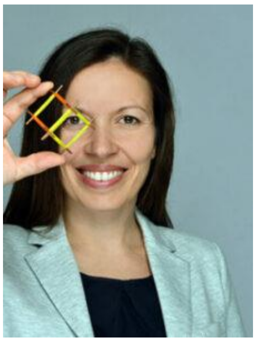

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Funding

This Symposium is supported by the **German Science Foundation** (DFG) through the **F^{3}G** research consortium for promoting equality at FAU Erlangen-Nürnberg. All participating initiatives are listed below:

- CRC 1452 CLINT - Catalysis at Liquid Interfaces
- CRC 1411 - Design of Particulate Products
- CRC 1540 - Exploring Brain Mechanics
- CRC Transregio 154 - Mathematical modelling, simulation and optimization using the example of gas networks
- CRC Transregio 306 QuCoLiMa - Quantum Cooperativity of Light and Matter
- CRC 1483 EmpkinS - Empatho-Kinaesthetic Sensor Technology – Sensor Techniques and Data Analysis Methods for Empatho-Kinaesthetic Modeling and Condition monitoring
- RTG 2861 - Planar Carbon Lattices
- RTG 2495 - Energy Conversion Systems: From Materials to Devices
- RTG 2475 - Cybercrime and Forensic Computing
- FOR 2886 PANDORA - Pathways triggering Autoimmunity and Defining Onset of early Reumatoid Arthritis
- FOR5134 - Solidification cracks during laser beam welding
- Graduate School in Advanced Optical Technologies
- Graduate School Engineering Advanced Materials
- GRK2599 - Fine-Tuners of the Adaptive Immune Response
- FRASCAL - Fracture across Scales - GRK 2423
- KFG 17: Alternative Rationalitäten und esoterische Praktiken in globaler Perspektive

The members of the Organizing Committee of WIS24 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 Royal Society of Chemistry and Nature Chemistry for providing poster and flash talk prizes for our symposium.

DFG Deutsche Forschungsgemeinschaft

FG3

CLINT Catalysis at Liquid Interfaces

CRC 1411

EBM

TRR 154

QuCoLiMa TRR 306

PCL RTG 2861

Energy Conversion Systems IGK 2495

Cybercrime and Forensic Computing Research Training Group 2475

FOR5134 HPC4HPP

SAOT

ENGINEERING OF ADVANCED MATERIALS GRADUATE SCHOOL

GRK2599 Fine-Tuners of the Adaptive Immune Response

FRASCAL GRK 2423

FOR2886 PANDORA Autoimmunity Inflammation

ROYAL SOCIETY OF CHEMISTRY

nature chemistry

Department of Chemistry and Pharmacy

General Information

Conference Venue

Chemikum, FAU Erlangen-Nürnberg
Süd (South) Campus Nikolaus-Fiebiger-Str. 10
91058 Erlangen

Photo: Conference Picture of WIS23

The *Chemikum* building at FAU is an ideal location for the symposium, since it houses several of FAU's chemistry departments. Fully equipped lecture halls ensure the realization of our symposium in a modern environment. It also offers ample room for the poster session, stimulating and inspiring further discussions. All lectures will take place in the lecture hall *C1*. Coffee breaks, lunch, and the poster session will be in and around the seminar room. Both rooms are located on the ground floor.

Transportation

Erlangen, Nürnberg, and Fürth are all connected using the **VGN transit system** (https://www.vgn.de/). Bus tickets can be purchased on the bus with cash or on the VGN app with debit/credit cards; train tickets can be purchased at one of the automatic machines at the station, on the **VGN** app, or the Deutsche Bahn (**DB**) app.

Airports

- Nürnberg Airport: To reach Chemikum, take the **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€). You can also take a taxi directly from the airport to Chemikum (approx. 30 min and 40-50 €)
- München airport and Frankfurt airport: (approx. 3 hours by train)

Public Transport

A single one-way trip within the Erlangen area, including to the FAU campus, costs 2.42€.

From Nuremberg: Take the **VGN Bus 30** (destination: "Erlangen Arcaden") 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" located on Bahnhofplatz, which is considered the city center of Erlangen.

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

- **Bus 287** (destination "Sebaldussiedlung"): Exit the bus at "Technische Fakultät", then walk approx. 5 min to Chemikum.
- **Bus 293** (destination "Bruck Bahnhof"): Exit the bus at "Sebaldussiedlung", then walk approx. 3 min to Chemikum.
- **Bus 295** (destination "Tennenlohe"): Exit the bus at "Erlangen Süd", then walk approx. 12 min to Chemikum.

Detailed Program

Monday, July 22nd

09:00 – 10:00	**Registration**
10:00 – 10:30	Welcome Address by the **Organizing Committee** and **Andrea Bréard** (FAU Erlangen-Nürnberg, DE)

Session 1 (Chair: Henry Dube)

10:30 – 11:20	**Keynote Lecture: Natalie Stingelin** (Georgia Tech, USA) *From the Swiss Mountains to Become Chair of the School of Materials Science and Engineering at the Georgia Institute of Technology: "Following Ones Dreams"*
11:20 – 12:00	**Invited Lecture: Ivana Fleischer** (University of Tübingen, DE) *I did it my way – breaking bonds and stereotypes*
12:00 – 13:15	**Lunch Break**

Session 2 (Chair: Ani Ozcelik)

13:15 – 13:55	**Invited Lecture: Anne M. Baranger** (UC Berkeley, USA) *Thriving in the College of Chemistry: Assessing and Improving Academic Culture*
13:55 – 14:05	**Flash Talk: Nath Mala** (Indian Institute of Technology Roorke, IN) *Nanocomposites, Ag/Mn_2O_3, As Efficient Heterogeneous Catalyst For Reduction Of Nitrophenols: Potential Wastewater Treatment*
14:05 – 14:35	**Invited Lecture: Ingrid Span** (FAU Erlangen-Nürnberg, DE) *Hydrogenases Made Crystal Clear*
14:35 – 16:05	**Coffee Break with Brain-Dating**

Session 3 (Chair: Sabine Maier)

16:05 – 16:45	**Invited Lecture: Marjan Zakerin** (Bosch, DE) *Seizing the Horizon: Empowering Women to Navigate and Triumph in Their Career Voyage*
16:45 – 16:55	**Flash Talk: Hemlata Agarwala** (Technical University of Munich, DE) *Photochemical CO_2 reduction to HCOOH by an organocobalt catalyst - Two different mechanisms with temporal evolution of catalysis, effectuated by second coordination sphere interactions*
16:55 – 17:25	**Invited Lecture: Carolin Müller** (FAU Erlangen-Nürnberg, DE) *Excited-State Odyssey: Charting Maps with Data-Driven Strategies*
19:30 -	**Speakers Dinner** (*upon invitation*) **Students Dinner** at Gaststätte mit Biergarten "Am Röthelheim" (*at own expenses, Am Röthelheim 40, 91052 Erlangen*)

Tuesday, July 23rd

Session 4 (Chair: Eugenia Pérez-Ojeda)

09:00 – 09:50	**Keynote Lecture: Patricia Hunt** (Victoria University of Wellington, NZ) *Exploring a Non-Polar Cope Rearrangement in (Polar) Ionic Liquids*
09:50 – 10:30	**Invited Lecture: Anelis Kaiser Trujillo** (Uni Freiburg, DE) *Sex/Gender in the Brain and Diversity in Neuroscience*
10:30 – 11:00	**Coffee Break**

Session 5 (Chair: Alejandro Cadranel)

11:00 – 11:40	**Invited Lecture; Magalí Lingenfelder** (EPFL, CH; Ikerbasque, ES) *From Tracking Atoms to Harnessing Electron Spin: Pioneering Pathways to Green Energy*
11:40 – 11:50	**Flash Talk: Lilli Reißenweber** (FAU Erlangen-Nürnberg, DE) *Directionality Reversal and Shift of Rotational Axis in a Hemithioindigo Macrocyclic Molecular Motor*
11:50 – 12:20	**Invited Lecture: Susanne Wintzheimer** (FAU Erlangen-Nürnberg, DE) *Supraparticles: Material design via nanoparticle assembly*
12:20 – 13:35	**Lunch break**

Session 6 (Chair: Peter Hommelhoff)

13:35 – 14:15	**Invited Lecture: Yu Jing** (Nanjing Forestry University, CN) *Rational Design of Two-Dimensional Organic Frameworks for Energy Conversion*
14:15 – 14:25	**Flash Talk: Inga Block** (University of Potsdam, DE) *Removal of organic contaminants from aqueous systems via adsorption onto spent coffee biochars*
14:25 – 15:05	**Invited Lecture: Katherine Geoghegan** (Springer Nature, UK) *Thinking outside the lab*
15:05 – 16:35	**Coffee Break with Round-Table Discussion** Discussion Leaders: **Ana-Sunčana Smith**, **Julien Bachmann** *Diversity and Inclusion in the Work Place, Positive Discrimination*

Session 7 (Chair: Dirk Guldi)

16:35 – 17:15	**Invited Lecture: Claudia Backes** (University of Kassel, DE) *Making nanomaterial inks from insoluble rocks- a personal journey*
17:15 – 17:25	**Flash Talk: Ashley Shin** (Max Planck Institute for the Science of Light, DE) *Ytterbium complexes with ultra-narrow absorption as atom-like molecular sensors*

17:25 – 17:35	**Flash Talk: Anika Höppel** (University Hospital Würzburg, DE) *Synthesis and characterization of magnesium phosphate supraparticles as coating components for bone implants*
17:35 – 19:30	**Poster Session**
19:30 -	**Dinner and Scientific Discussions**

Wednesday, July 24th

Session 8 (Chair: Danijela Gregurec)

09:00 – 09:50	**Keynote Lecture: María Dolores Pérez Meirás** (CIQUS-USC, ES) *Crafting nanographenes and nonconventional carbon nanostructures with an aryne-based “molecular Lego”*
09:50 – 10:00	**Flash Talk: María Lago Silva** (CIQUS-USC, ES) *Mechanically Interlocked Macromolecular Gears: Modulating Chiral Polymeric Helices with Rotaxane Pendant Groups*
10:00 – 10:40	**Invited Lecture: Ute Resch-Genger** (BAM, DE) *A Journey in Science – From a Graduate Student in Physical Chemistry to Head of Division Biophotonics*
10:40 – 11:00	**Coffee Break**

Session 9 (Chair: Karl Mandel)

11:00 – 11:40	**Invited Lecture: Sofia Dembski** (Fraunhofer ISC Würzburg, DE) *Gut Feeling and Intuition - My Personal Journey from Dentistry to Biomaterials*
11:40 – 11:50	**Flash Talk: Anna Zieleniwska** (Technical University of Munich, DE) *Balancing Act: The Dual Role of Heat Generation in Protein-Based Materials*
11:50 – 12:00	**Flash Talk: Hanfeng Zhou** (University of Dresden, DE) *Ions Selectively Intrigued Ionologic Devices for Logic Operation*
12:00 – 12:30	**Invited Lecture: Dagmar Fischer** (FAU Erlangen-Nürnberg, DE) *Sustainability and green concepts in pharmaceutical nanoformulations*
12:30 – 12:50	**Award Ceremony and Closing Remarks**
12:50 –	**Lunch and Farewell**
14:00 –	**Graduate School EAM Get-Together** *(register online in advance)*

Keynote and Invited Speakers

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Abstracts

Keynote Speakers

Exploring a Non-Polar Cope Rearrangement in (Polar) Ionic Liquids

Prof. Patricia Hunt[1]

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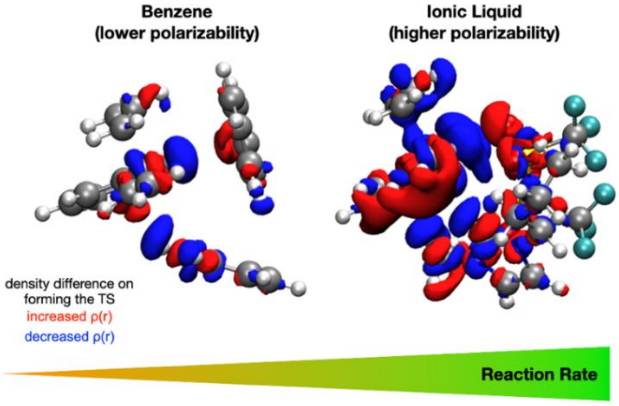
Ionic liquids (ILs) are a novel class of solvent composed entirely of ions that are (typically) liquid below 100ºC. The ions are larger and more chemically complex than traditional molten salt ions. As a group ILs exhibit a variety of properties which set them apart from traditional molecular liquids. Many ILs are non-volatile, non-flammable, conductive, have good solubility / miscibility characteristics and exhibit a high thermal stability. These characteristics make ILs re-useable, and lead to ILs being considered as green reaction solvents. However, critically, we still lack a robust molecular level understanding of how ILs impact reactivity.

The impact of ionic liquids on polar reactions is well recognised, however the impact of ILs on non-polar reactions is less well explored. Pericyclic Cope rearrangements are highly concerted, exhibit minimal charge localisation and pass through an uncharged but structurally well-defined transition state, and thus provide a good mechanism for exploring the impact of IL polarity/polarizability on chemical reactivity. Recently, a 10x rate enhancement has been observed for the Cope rearrangement of hexa-1,5-dien-3-ylbenzene in the IL 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)-imide [C_4C_1im][NTf_2] compared to benzene.[1]

Why this non-polar Cope rearrangement is substantially accelerated within a (polar) IL is not obvious. We have undertaken a DFT based computational study of the hexa-1,5-dien-3-ylbenzene Cope rearrangement comparing molecular solvents with the IL [C_4C_1im][NTf_2].[2] We have evaluated a volume of activation and identified two potential volume effects that could contribute to the rate enhancement. Specific solvent interactions for benzene and the IL are also explored. We find that the IL ions can form a Van der Waals pocket in which the TS sits, and that the TS electron density can be significantly more polarised for the IL. Overall, we provide a deeper molecular level insight into the impact of ILs on non-polar reactions.



References

[1] S. Keaveney, R. Haines, and J. Harper, *ChemPlusChem* **2017**, *82* (3), p449–457, doi 10.1002/cplu.201600585
[2] G.Smith, S. Koutsoukos, B. Lancaster, J. Becker, T. Welton and P.A. Hunt, *Phys. Chem. Chem. Phys.,* **2024**, 26, 12453-12466, doi: 10.1039/ D4CP00156G.

Crafting nanographenes and nonconventional carbon nanostructures with an aryne-based “molecular Lego”

Dolores Pérez[1]

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The discovery of graphene and other carbon-based materials opened a new era in materials science, wherein synthetic organic chemistry is called to play an important role. In particular, the tailored, bottom-up synthesis of nanosized graphene substructures (nanographenes) and other polycyclic conjugated hydrocarbons (PCHs) with customized shapes and electronic properties, is a very active area of research. Within this realm, aryne intermediates stand out as ideal synthetic building blocks, providing privileged strategies for the convergent construction of polycyclic compounds containing aromatic rings.[1,2]

In this lecture, some recent contributions from our group to this field will be presented, with particular emphasis on the use of polycyclic arynes and bisaryne precursors for the straightforward access to extended and/or structurally complex aromatic architectures. Our efforts towards the synthesis of singular aromatics and relevant π-functional materials, such as acenes, cycloarenes, porous nanographenes or novel fullerene derivatives will be showcased, including selected examples resulting from the successful combination of solution-phase chemistry based on aryne cycloaddition reactions, with the on-surface transformation of the thus-prepared polycyclic precursors.

During my presentation, I will aim to contextualize my aforementioned current research work within the broader framework of my scientific and academic trajectory. This will include not only my scientific training and research path, but also my role as a founder and co-director of CiQUS, a young research center which over the span of just 12 years, has evolved into one of the leading European university institutes working at the interdisciplinary intersection of chemistry, biology, and materials science.

References

[1] F. García, D. Peña, D. Pérez, E. Guitián, in *Modern Aryne Chemistry*, Wiley-VCH, 27-68 (2021).
[2] I. Pozo, E. Guitián, D. Pérez, D. Peña, *Acc. Chem. Res*., **2019**, *52*, 2472-2481.

From the Swiss Mountains to Become Chair of the School of Materials Science and Engineering at the Georgia Institute of Technology: “Following Ones Dreams”

Natalie Stingelin[1]

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An overview of my journey is given, growing up in a small Swiss mountain town, to becoming a student at ETH Zurich, postdoc at Cambridge University, researcher at Philips Research in Eindhoven, to Professor, first in London, then across the globe in Atlanta – all propelled by scientific curiosity and the desire to educate. Examples of my research to turn around the reputation of plastics are also delivered, presenting research into ‘cool’ polymers for cars and buildings aimed to reduce the need for air conditioning and improve energy efficiency. Whilst there is significant potential in environmental applications of these materials, efforts are still required to design plastics of desired functions. Clearly, the idea that plastics could play a big part in a more sustainable future world might seem far-fetched, with seabirds trapped in multipack drink rings, and mid-ocean islands of indestructible rubbish, however, here it is shown that new smart plastics may yet rescue the reputation of this all-consuming 20th and 21st century material.

Invited Speakers

Making nanomaterial inks from insoluble rocks- a personal journey

Claudia Backes[1]

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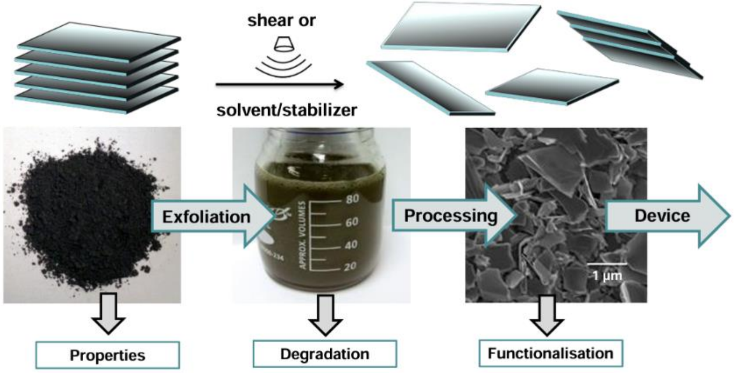
In this talk, I will review my personal scientific journey which began during my PhD time at the University of Erlangen-Nürnberg in 2007, i.e. at a time, when single-walled carbon nanotubes were intensely investigated worldwide. These nanomaterials consist of an all sp^2-carbon framework just like graphite, but rolled up into hollow cylinders. Depending on the way they are rolled up, they have different electronic properties, e.g. metallic or semiconducting. This completely fascinated me and I found my first scientific love. Since they are insoluble rocks, I worked on efficient ways to "solubilize" them and then potentially separate them. During this time, it also became clear that a single layer of graphite termed graphene is yet another high potential wondermaterial so that a lot of research activities moved from nanotubes to the two-dimensional (2D) objects. Here, similar problems arise: the abundant starting point to 2D materials are natural stacks of the layers - which are again insoluble rocks. However, using the learnings from carbon nanotubes, it was demonstrated by a team of researchers at Trinity College Dublin, that individual layers of graphite can be peeled off to produce graphene in a process now termed liquid phase exfoliation. Even though I had already been working in science administration at the Cluster of Excellence "Engineering of Advanced Materials", I was fascinated by this development and strongly encouraged by the people in my environment to do a postdoc. I therefore joined the researchers in Dublin in 2012 on the exciting quest to optimize and understand this exfoliation process in liquids. Some of our research activities today still focus on fundamentally understanding the mechanism of the material production. While working in Dublin, 2D materials in general were more and more in the scientific spotlight, as many materials are layered and can be exfoliated in similar ways. This extremely rich playground of materials is the origin of a hype that now lasts well over a decade. In my career development, I strongly benefitted from this and all opportunities that came with it. In 2015, I established my independent junior research group at Heidelberg University and became Chair Professor at Kassel University in 2021 focusing on exfoliation, processing, characterisation and chemical modification of a range of 2D materials.



Thriving in the College of Chemistry: Assessing and Improving Academic Culture

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The Department of Chemistry at UC Berkeley has undertaken a multiyear effort to create an inclusive academic research culture. In an initiative led by graduate students a department-tailored academic climate survey has been developed, which provides quantitative evidence that forms the foundation of annual community discussions between graduate students and faculty.[2] Participation of leadership, faculty, students, and staff have led to a coordinated set of interventions being put in place.[3] Longitudinal assessment indicates a shift in the perception of the academic climate. Using frameworks of belonging and social influence to guide our understanding that alignment of values is important for inclusion and belonging, questions probing faculty, graduate student, and postdoc values and perceptions of values were included on the survey. The results showed that students who perceived better alignment of values were also more likely to indicate they were excited to remain in the discipline. In response to community discussions, we have created a short course to promote discussions of the complexity of the impact of the discipline of chemistry on diverse communities and the responsibility scientists have in the discipline. Development and assessment of the climate survey and short course, along with recent work to extend these methods to undergraduate populations will be presented.

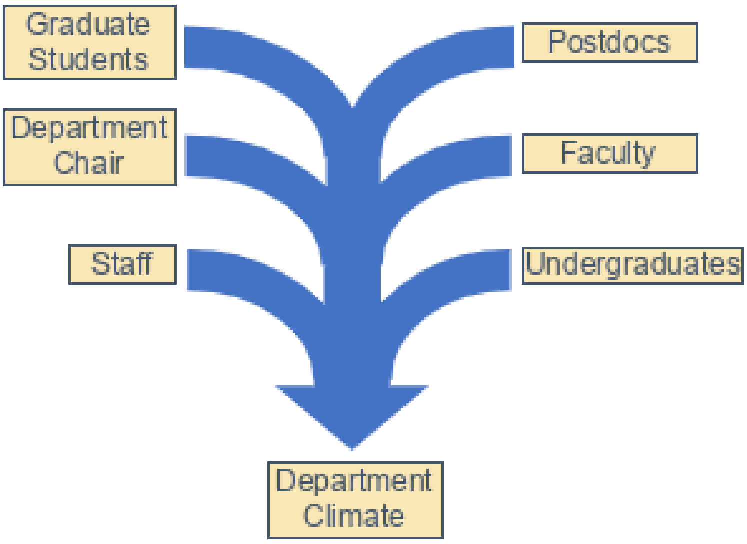

Figure 1. Improved department climate is the result of contributions from all members of the community.

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Gut Feeling and Intuition - My Personal Journey from Dentistry to Biomaterials

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It is great to have personal plans and dreams for your professional carrier. They are very important and helpful: they give us direction, framework and security. They motivate us and help us achieve our goals.

But what happens when things don't go as planned? Should we give up, change or refocus our goals or make a total restart?

I strongly believe that instead of giving up, getting frustrated and crying over what doesn't work out, we should keep our eyes open and be ready for new opportunities. Because there is always a new door opening somewhere.

We should listen to our gut feeling and consider adjusting our plans and strategies based on what we learn. Sometimes intuitive decisions can lead to unexpected opportunities and success.

I want to share with you my personal experience with the planning and intuitive processes and the decisions arising from there. I will tell you how it led me, a young Russian woman with a degree in dentistry, to become a chemist in Germany and finally the deputy director of the Translation Center of Regenerative Medicine. My personal journey has led me to the exciting interdisciplinary world of our department. Here, we are not only researching and developing new materials for biomedicine and lab automation but e.g., also new cell-based tissue models as alternatives to animal testing.

Sustainability and green concepts in pharmaceutical nanoformulations

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Current trends in pharmacy turned to sustainability and green concepts leading to a re-thinking of the classical drug formulation techniques to avoid hazards for human health and the natural environment. The formulation of active substances by nanoparticle approaches has resulted in a high number of reports with new concepts and trends for the development and optimization of new drug carriers with varying architectures and novel carrier materials, but sustainability concepts are still rare.

The different steps and excipients for the preparation of polymer-based nanoparticles by nanoprecipitation and nanoemulsification as the most commonly used manufacturing techniques will be evaluated regarding sustainability [1]. New green and sustainable solvents are presented as alternatives for organic solvents to dissolve the polymers and the correlation between physicochemical solvent characteristics and the type of the formulation process, the particle characteristics, as well as effects on biological efficacy and toxicity are highlighted [2]. Alternatives for surfactants and emulsifiers will be discussed.

Additionally, the potential of natural polymers that are produced by organisms like bacteria or Archaea, as drug delivery systems will be presented such as bacterial nanocellulose used as wound dressings and lipidic archaeosomes for oral vaccination [3].

Conclusively, new excipients are available that present a significant advancement as green and sustainable alternatives in nanoparticle formulations and provide access to high-quality delivery systems with reproducible quality.

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I did it my way – breaking bonds and stereotypes

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It the research part of the talk, an overview on research activities of the Fleischer group will be given. Our research interests focus on development of new metal-catalyzed methods for the synthesis and use of sulfur-containing compounds, such as thioesters and thioethers. They constitute valuable synthetic intermediates and target compounds for material chemistry and pharmaceutical applications.[1] Our aim is to develop efficient transformations employing non-precious metals as homogeneous catalysts and to gain mechanistic understanding of the processes.

We have demonstrated the usefulness of thioesters in cross coupling reactions with arylzinc reagents to generate ketones (Figure 1a).[2] A defined nickel complex was employed as catalyst and a series of functionalized ketones was successfully obtained. The scope was later expanded to the coupling of thioesters with more reactive organomanganese reagents upon iron catalysis.[3]

Furthermore, we have developed nickel-catalyzed coupling reactions of challenging aryl chlorides and triflates with thiols, whereby max. TOF of 800 h^{-1} was achieved (Figure 1b).[4] A broad scope of substrates containing various functional groups and heterocyclic motifs was successfully converted. A systematic study of couplings of sterically hindered aliphatic thiols was conducted and accompanied by mechanistic studies.

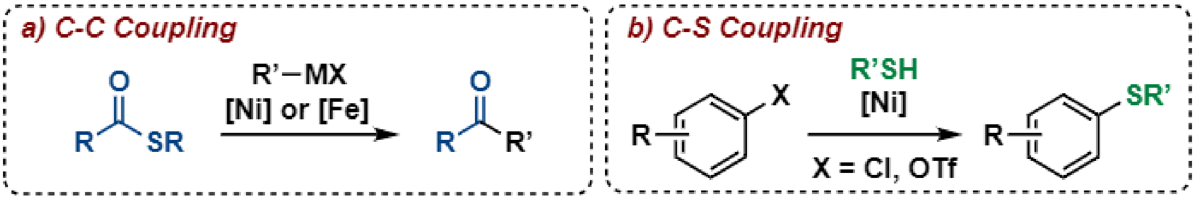

Figure 1. Examples of developed catalytic transformations of thioesters and thiols.

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Thinking outside the lab

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After completing a chemistry PhD, the typical paths available are to either continue with academic research — usually beginning with post-doctoral studies — or to join the industrial workforce. Both avenues maintain active laboratory research, so what are the paths for those of us who no longer want to be in the lab, but are still enthralled by the world of chemistry? Towards the end of my PhD, I began to consider other options that would keep me in the field I'd been studying for almost a decade but without getting my hands dirty, so to speak. This is when I discovered careers focused on the dissemination of scientific research – an area I had taken for granted until that point. My talk will discuss my journey to becoming a Senior Editor at Nature Chemistry while also discussing the role itself, which will include the process of publication at Nature Chemistry, how decisions are made, and tips to keep in mind when writing a research article.

Figure 1. From childhood to PhD and beyond. © M-H Jeeves[1]

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Rational Design of Two-Dimensional Organic Frameworks for Energy Conversion

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Two-dimensional (2D) metal-loaded organic frameworks (MOFs) have a high specific surface area, adjustable structural composition and uniform surface active sites, making them ideal catalysts for energy conversion. However, the large pore structure limits the effective transmission of electrons. Designing 2D MOFs with high stability and high conductivity is the key to obtaining an efficient electrocatalyst.[1] By performing first principles calculations, we designed a series of 2D MOFs by coupling conjugated organic ligands with four-coordinated transition metals, and applied them to various electrocheimcal reactions, including oxygen reduction reaction, oxygen evolution reaction, nitrogen reduction reaction and carbon dioxide reduction reaction.[2,3] The computational results show that variation of metals and coordination environments can not only allow the formation of stable d-π conjugated structures, but also enable the adjustment of catalytic activity. The designed 2D MOFs with Co centers exhibit higher electrocatalytic activity than traditional precious metal catalysts. With the help of the state-of-the-art methods, we revealed the relationship between lattice, composition and catalytic activity,[4] providing rationale for the design of effective catalysts for energy conversion.

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From Tracking Atoms to Harnessing Electron Spin: Pioneering Pathways to Green Energy

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The journey from the simple desire to “see atoms” to the exploration of the electron spin for green energy applications reflects a path of profound advancements in our understanding of the atomic and subatomic world over the past decades. These advancements are not only intellectually satisfying but also hold the potential to address critical global challenges, such as sustainable energy.

In our research group, we tackle the challenge of sustainable energy by creating customized nanostructured materials that draw inspiration from nature (biomimicry), integrating fundamental principles from interfacial chemistry and surface physics. For this presentation, I draw inspiration in the process of photosynthesis for the design of earth-abundant materials that drive electrocatalytic energy conversion processes: such as CO_2 electroreduction and water splitting.

The use of cutting-edge scanning probe microscopy enables us to visualize dynamic electrochemical processes at the nanoscale through in-situ imaging [1]. The detailed atomic-scale information we gather inspires us to explore further: to use unconventional strategies that harness electron spin to enhance electrocatalytic conversion processes [2-4]. This innovative approach has allowed us to develop state-of-the-art materials that are two to three times more efficient in electrocatalysis [3-4].

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Excited-State Odyssey: Charting Maps with Data-Driven Strategies

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Photochemistry offers a promising route to sustainable chemical processes. However, to exploit its full potential, it is necessary to explore the potential energy landscapes of different excited states. This exploration resembles an odyssey, because in the absence of design principles and detailed structural information for excited states, detailed maps for these surfaces are lacking.

Quantum chemical simulations provide glimpses on these landscapes, yet their accuracy is hampered by computational costs associated with quantum chemical methods, restricting their use to small systems (*e.g.*, ≤100 atoms) and short timeframes (ranging from femto- to picoseconds). Here, data- and science-driven strategies emerge as a guiding force. For example, by leveraging existing quantum chemical data across various molecular configurations and excited states, machine learning approaches can accelerate photodynamics simulations to navigate the excited state manifold or drive static approaches to localize critical points on various excited-state surfaces.

This presentation provides an overview of how machine learning can streamline the charting of maps for the landscape of photochemical reactions involving various excited states. Introducing the machine learning method, **SPaiNN** [1], and its companion database, **SHNITSEL** [2,3], we delve into a promising duo driving the exploration and prediction of excited-state landscapes. **SHNITSEL** serves as a comprehensive repository housing computational data for various photochemical reactions, meticulously crafted as the **S**urface **H**opping **N**ewly **I**nvented **T**raining **S**et for **E**xcited-state **L**earning. Specialized in training and predicting excited state properties, **SPaiNN** will be showcased using examples from the **SHNITSEL** database, marking the commencement of an Excited-State Odyssey, charting maps with data-driven strategies.

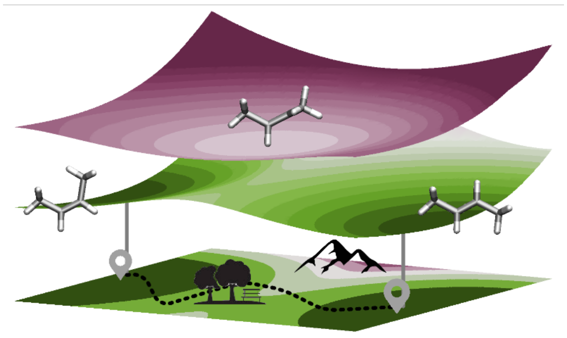

Figure 1. Schematic illustration of the excited state map of buten.

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Hydrogenases Made Crystal Clear

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Hydrogenases are highly efficient metalloenyzmes for hydrogen generation. [FeFe] hydrogenases are highly active and biased toward hydrogen production, but they are also highly sensitive to oxygen. We focus on studying the enzyme from *Desulfovibrio desulfuricans*, because it can adopt a state, in which the active site is protected from degradation by oxygen. We combine X-ray crystallography with single-crystal spectroscopy to understand how the enzyme protects itself from oxygen and to elucidate the catalytic mechanism.

Sex/Gender in the Brain and Diversity in Neuroscience

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Brain research attracts significant scientific and public interest. For a long time, neuroscientific publications have explored why women and men feel, think, act, or speak differently. Today, the questions surrounding sex/gender in neuroscience have become more complex, incorporating concepts of diversity, intersectionality, and gender identity. AI-based methods, with their underlying emphasis on multiplicity, further highlight human diversity. What do these developments mean for questions of sex/gender in neuroscience and equality in STEM? Despite advancements, the gender pay gap in STEM persists, and the number of women in certain STEM fields has remained unchanged for nearly 30 years. This presentation aims to prompt reflection on these potential connections and critically examine our own research.

Supraparticles: Material design via nanoparticle assembly

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In the past decades, tremendous effort has been made in synthesizing nanoparticles because of their unique size-related properties. In the last 15 years, a step further has been taken considering nanoparticles as building blocks[1] and creating more complex particulate units from them, i.e. supraparticles (Figure 1a). Such entities not only conserve nanoparticulate properties, while lifting the particle sizes to the microscale range but also provide additional functionalities exceeding the sum of properties of their constituent building blocks.[2] This talk highlights the potential of spray-drying as an assembly process of colloidal nanoparticles to create supraparticles.[3] In this process, the confined space within a liquid droplet is reduced upon drying, forcing its ingredients to come together (Figure 1b). Thanks to the design of the supraparticulate architecture and composition new functionalities emerge opening up their use in diverse applications.[4] As examples, spray-dried supraparticle-based optical hydrogen sensors[5] and heterogeneous catalysts[6] containing catalytically active liquid phases will be shown. Altogether, it will be demonstrated that spray-drying is a very interesting and powerful tool for materials chemists to enable the scalable design of hybrid materials.

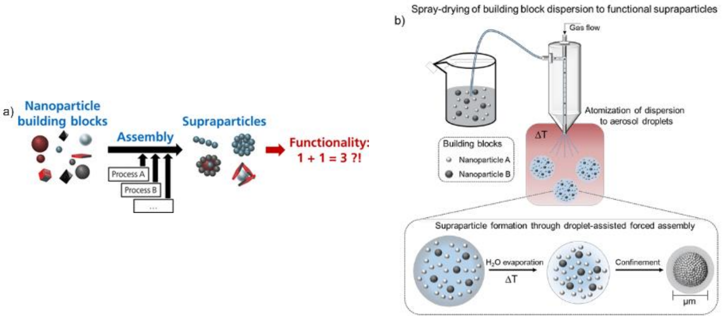

Figure 1: a) Unexpected functionalities emerge from an assembly of nano building blocks to supraparticles.[2] b) The spray-drying process of a binary nanoparticle dispersion and the forced assembly of these nanoparticles during droplet evaporation resulting in supraparticles.[6]

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Seizing the Horizon: Empowering Women to Navigate and Triumph in Their Career Voyage

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As I approached the end of my postdoctoral program, the quest for an industry position unfolded like an intensive self-improvement workshop. The first step was to distill my academic achievements and accomplishments into an industry-standard CV—a document that would speak to the needs and language of the corporate world. This task alone was akin to enrolling in an advanced class of self-discovery and skill articulation.

The learning curve steepened as I attempted to decode the labyrinth of job titles. Each title carried with it a unique set of tasks and expectations, often obscured by industry jargon. To unravel these mysteries, I reached out to professionals on LinkedIn for informational interviews. These conversations were invaluable, granting me insights into the day-to-day realities of the roles I aspired to and teaching me how to communicate my capabilities in terms that resonated with industry recruiters.

But the journey didn't stop at linguistic mastery. The art of networking became my lifeline. It was through a relentless cycle of job applications, digital networking, attendance at industry events, and the cultivation of relationships with seasoned industry mentors that I began to see progress. These connections not only provided guidance but also served as conduits to potential opportunities.

In retrospect, I recognize that this phase was a comprehensive lesson in self-awareness and professional development. It exposed gaps in my PhD and postdoctoral training—areas where the development of practical soft skills, and industry-relevant skills was overlooked. It was a strong reminder that the academic community, while nurturing intellectual growth, often does not prepare one for the pragmatic aspects of career starting and advancement in the industry.

This reflection on the insights gained, which I am keen to share with you, extends beyond a mere personal account. It serves as a rallying cry for academic institutions. It underscores the importance of tailored programs that equip scientists, particularly female scientists, to navigate the predominantly male-dominated industrial sphere. These programs ensure that the transition from academia to industry is not a mere leap, but rather a well-supported stride toward a fulfilling and rewarding career. Recognizing that the strategies and methods that have brought us to our current juncture may no longer be effective for the challenges ahead, I am poised to propose a comprehensive pragmatic success model. This model is not only theoretically sound but also pragmatically viable, tailored to meet the demands and nuances of both the academic and industrial landscapes.

Flash Talks

Photochemical CO_2 reduction to HCOOH by an organocobalt catalyst - Two different mechanisms with temporal evolution of catalysis, effectuated by second coordination sphere interactions

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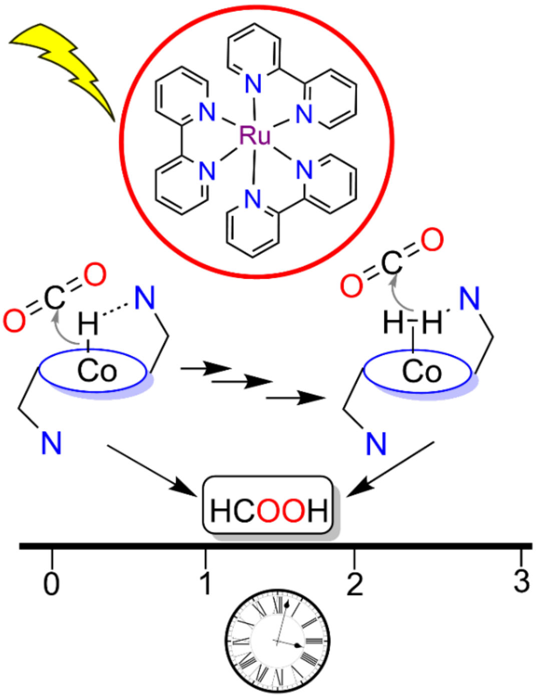
Photochemical reduction of CO_2 to formic acid (HCOOH) using molecular transition metal complexes as catalysts has been previously documented to proceed *via* either of the two mechanisms: CO_2 insertion into metal hydride bonds, or hydrogenation of CO_2. This presentation highlights the photoreduction of CO_2 to HCOOH that adopts both these pathways by a single monometallic molecular catalyst featuring earth-abundant cobalt - a characteristic not observed in other molecular catalysts for CO_2 photoreduction to date. This dual functionality stems from distinctly different, active forms of the catalyst, at different temporal stages of irradiation. *in situ* NMR spectroscopy sheds light on the potential catalytic intermediates at various time points of irradiation by visible light. These observed states align with the kinetic profiles of product evolution, proving instrumental in revealing the catalyst's unique behavior.



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This content is a preprint and has not been peer-reviewed.

Removal of organic contaminants from aqueous systems via adsorption onto spent coffee biochars

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Nowadays, cleaning (waste)water from organic and inorganic pollutants is becoming more and more relevant due to the growing scarcity of clean water. In our research we focus on the reuse of spent coffee grounds (SCG) for the making of biochars which then can be applied in water purification via adsorption. [1] SCG present a cheap and abundant waste material, which can be converted to activated carbon via various treatment methods in a pyrolysis process. The resulting carbon materials show great adsorption capacities during experiments in single-contaminant solutions as well as in mixtures for all kinds of organic pollutants. Also, in the attempt for better recyclability of materials magnetic biochars are in development. Our main focus currently is on the adsorption of the dyes methylene blue and methyl orange, the pharmaceuticals diclofenac and tetracycline as well as on the endocrinic disruptor bisphenol A.

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Synthesis and characterization of magnesium phosphate supraparticles as coating components for bone implants

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Biomedical implants have shown great promise as bone tissue replacement in recent decades. To enhance implant bio-integration and the healing process, bioactive ceramic coatings have been developed. In this context, magnesium phosphate (MgP) has received great attention due to its high biodegradability, osteoconductivity and the use as drug carrier, but research is still limited.

Here, we present our recent activities of MgP supraparticles to improve the properties of bone implant coatings while providing antibacterial properties. MgP NPs were prepared by a sol-gel process followed by spray drying together with antibacterial Cu ions into supraparticles.[1,2] First coating experiments with Cu-doped MgP supraparticles were done on Ti substrates by a suspension flame spraying process. In a second approach, to test the biocompatibility of MgP and the possible cytotoxicity of Cu, cell viability assays were performed and the antibacterial effect of Cu was determined.

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Mechanically Interlocked Macromolecular Gears: Modulating Chiral Polymer Helices with Rotaxane Pendant Groups

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Nature uses the bottom-up approach to create complex systems involved in processes such as signaling or the transmission of chiral information.[1] A small part of such complex systems usually undergoes a change in its conformational composition. This response is then effectively transmitted to the rest of the system through a conformational communication mechanism. In this work, we show how combining mechanically interlocked macromolecules, such as a chiral rotaxane used as a pendant, with a helical polymer, such as a poly(phenylacetylene) (PPA), it is possible to create a macromolecular gear in which the motions in the mechanically interlocked macromolecules used as pendants are amplified by changes in the backbone of the helical polymer. Therefore, this work demonstrates how the fields of molecular machines, supramolecular chemistry, and polymers can work together to create complex systems and shows how information can be effectively transferred across different levels of complexity.

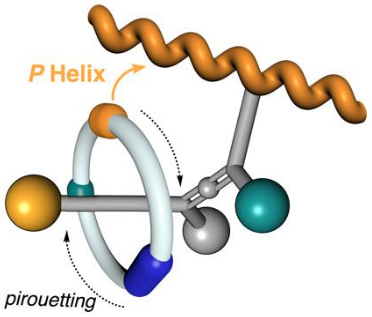

Figure 1. Schematic representation of a macromolecular gear

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Nanocomposites, Ag/Mn_2O_3, As Efficient Heterogeneous Catalyst For Reduction Of Nitrophenols: Potential Wastewater Treatment

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Metal/Metal oxide nanocomposites gained importance due to their application in supercapacitors, wastewater treatment, and energy storage. A single step thermal decomposition method was used to synthesize Mn_2O_3 nanoparticles. Further, three Ag/Mn_2O_3 nanocomposites were synthesized with different amounts of Ag, represented as AM-5 (5% Ag), AM-10 (10% Ag), and AM-15 (15% Ag), and characterized by various techniques. Their application for the wastewater treatment was investigated for catalytic reduction of nitrophenols (NPh)in presence of $NaBH_4$ by employing different amounts of all the synthesized materials along with varying amounts of $NaBH_4$, and 4-nitrophenol's (4-NPh). AM-15 was the, most effective catalyst as it reduced 4-NPh in 6.5 min, whereas AM-10 and AM-5 reduced 4-NPh in 8 and 11 min, respectively. The order of reduction of different nitrophenols:3-NPh > 4-NPh > tri-NPh > 2-NPh by using 30 μL of AM-15 (from the suspension contains 1 mg/mL). AM-15 efficiently reduced a real industrial sample-dye-bath effluent and EFF (a simulated industrial sample). Reusability of AM-15 for reduction of 4-NPh is excellent up to five cycles.

Directionality Reversal and Shift of Rotational Axis in a Hemithioindigo Macrocyclic Molecular Motor

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Molecular motors are central driving units for nanomachinery and control of their directional motions is of fundamental importance for their functions.[1] Light-driven variants use an easy to provide, easy to dose, and waste free fuel with high energy content, making them particularly interesting for applications. Typically, light-driven molecular motors work via rotations around dedicated chemical bonds where directionality of the rotation is dictated by the steric effects of asymmetry in close vicinity to the rotation axis.[2] In this work we show how unidirectional rotation around a virtual axis can be realized by reprogramming a molecular motor. To this end, a classical light-driven motor is restricted by macrocyclization and its intrinsic directional rotation is transformed into a directional rotation of the macrocyclic chain in the opposite direction. Further, solvent polarity changes allow to toggle the function of this molecular machine between a directional motor and a non-directional photoswitch. In this way a new concept for the design of molecular motors is delivered together with elaborate control over their motions and functions.

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Ytterbium complexes with ultra-narrow absorption as atom-like molecular sensors

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In quantum technologies, the energetic disorder induced by a fluctuating liquid environment acts in direct opposition to the precise control required for coherence-based sensing. Overcoming fluctuations requires a protected quantum subspace that only weakly interacts with the local environment, especially in sensor applications. In this work, we explore a Yb^{3+} complex, (thiolfan)YbCl(THF), that exhibits an extraordinarily narrow absorption linewidth in solution at room temperature with a full-width at half-maximum of 0.625 eV.[1] At 77 K, a spectral hole burning measurement was performed to resolve an even narrower linewidth of 410 peV in disordered glass. A combination of density functional theory and multireference methods match experimental transition energies and oscillator strengths, illustrating the role of spin-orbit coupling and asymmetric ligand field in enhancing absorption in lanthanide complexes. Narrow linewidths allow for a demonstration of extremely low-field magnetic circular dichroism at room temperature, employed to sense weak magnetic fields, down to Earth scale. We term this system an ‘atom-like molecular sensor’ (ALMS) and explore its capabilities toward liquid-phase quantum sensing.

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Ions Selectively Intrigued Ionologic Devices for Logic Operation

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Ion-electroadsorption devices based on electrical double layer capacitors (EDLCs) present a new avenue for energy efficient ion-based computing. Especially, capacitive analogues of semiconductor-based diodes (CAPodes) with high rectification ratio are attractive for a great number of technological applications, such as logic gates. High rectification ratios render CAPodes attractive for a great number of technological applications, from energy storage to alternating current (AC) rectification and logic gates. Here, we disclose the general concepts for bias-direction-adjustable n- and p-CAPodes achieved by selective ion sieving. Controllable-unidirectional ion flux is realized by blocking electrolyte ions from entering sub-nanometer pores, leading to an efficient sieving effect at pore size below the size of bulky cations or anions. A precise regulation concept can effectively balance the current between positive and negative bias. The resulting CAPodes exhibit charge-storage characteristics with a high rectification ratio (RR_{II}, 96.29%). The enhancement of capacitance is attributed to the high surface area and porosity for our proposed omnisorbing carbon, leading to a larger ion-accessible pore space that enables rapid charge storage kinetics. Furthermore, we demonstrate the use of an integrated device in a logic gate circuit architecture to implement ‘OR’ logic operations. This work demonstrates CAPodes as a generalized concept to achieve p-n and n-p analogue junctions based on selective ion electrosorption, illustrates the enormous diversity and complexity attainable in CAPode systems, provides a comprehensive understanding and highlights applications of ion-based diodes in ionologic architectures.

Balancing Act: The Dual Role of Heat Generation in Protein-Based Materials

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Heat generation in protein-based materials presents both challenges and opportunities, embodying a dual role that significantly impacts their applications. This talk delves into the intricate balance between the beneficial and problematic aspects of thermal effects in protein-derived materials. Controlled heat generation can be used for energy harvesting. Conversely, excessive or uncontrolled heat can lead to material degradation, loss of structural integrity, and reduced performance, posing significant obstacles for practical implementations.

We will elucidate our approach to decoding the underlying mechanisms of heat generation in these materials, examining how molecular interactions and structural properties influence thermal behavior. Additionally, we will demonstrate how precise thermal management can transform potential drawbacks into advantageous features, thereby optimizing material performance. By understanding and manipulating heat generation, we can unlock new possibilities for protein-based materials, enhancing their versatility and efficiency. This presentation provides an overview of current research, highlights emerging trends, and proposes strategies for balancing beneficial and detrimental thermal effects.

Poster Presentations

Positively charged Au-Fe_3O_4 nanoparticle in Immune therapy

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This study presents the synthesis and functionalization of Au-Fe_3O_4 nanoparticles using two distinct methods to control their size, shape and magnetic properties. The first method, termed the nanoheterodimers nanoparticle approach, involves the thermal decomposition of an iron(III)precursor on pre-synthesized gold nanoparticles. In the second method, known as patchy nanoparticles, Au-Fe_3O_4 nanoparticles are synthesized by adding gold acid, iron(II)salt and mercapto carbon-acid into an ammonia solution.[1, 2] Each nanoparticle was functionalized with various positively charged ligands (e.g. biotin, penicillamine, polyethylene imine, dopamine). These positively charged nanoparticles can bind to the negatively charged backbone of siRNA. The nanoparticles transport the siRNA into immune cells to downregulate the expression of the PD-1 receptor through RNA interference. [3]

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Synthesis and Characterization of NBD-HBC Conjugates for non-conventional Data Storage

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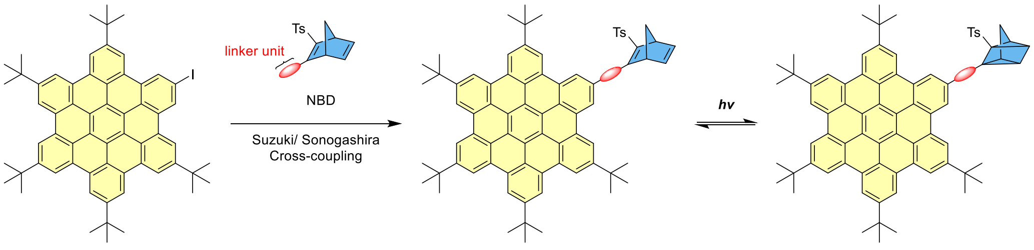
Due to non-zero band gap and high extended π-system hexa-*peri*-hexabenzocoronene (HBC) has received promising abilities in molecular electronics and photo optics.[1] Furthermore, functionalization of the HBC core with photo-optical molecules provided novel molecular devices with improved opto-electronic properties.[2] In contrast, photo-switches as norbornadiene (NBD) were intensively investigated in molecular solar thermal (MOST) energy storage.[3] Thereby, NBD can be converted into its valence isomer quadricyclane (QC) by absorbing light. It is intuitive to assume that the synthesis of such hybrids provides highly interesting opto-electronic devices that can possibly isomerize by light absorption. For this purpose, HBC-NBD conjugates are synthesized by Suzuki or Sonogashira cross-couplings incorporating possible linkers as benzene or ethynyl. Furthermore, the ability of these HBC-NBD conjugates to switch to its valence isomer HBC-QC are analysed in photo-studies.



HBC

HBC - NBD

HBC - QC

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Artificial Cobalt-Substituted Metalloenzymes

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Iron-sulfur clusters are among the most ancient cofactors in proteins and play important roles in many biological processes, including electron transfer reactions such as hydrogen evolution.[1], [2] Iron is readily oxidized, which destroys the cluster and inactivates enzymes.[3] Unnatural metallic cofactors may convey stability and maintain enzymatic activity. Cobalt was reported to form similar clusters [4] and cobalt-containing complexes were shown to catalyze hydrogen evolution and water-splitting reactions.[5] These artificial clusters can be incorporated into proteins by chemical reconstitution, semi-enzymatic maturation, or *in vivo* assembly. The successful production of artificial metalloproteins is investigated for proteins with metal centers of different nuclearities. Here we report the efficacy of cobalt incorporation in model proteins of three different host organisms for each level of cluster complexity.

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Synthesis and Characterization of Donor-Acceptor Windmill HBCs

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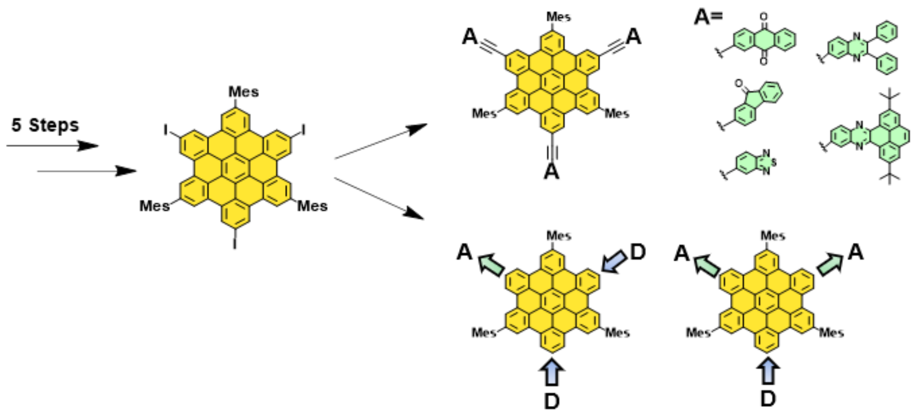
The investigation of graphene related compounds with non-zero band gaps, such as Hexa-*peri*-hexabenzocoronene (HBC), became of major interest in recent years. [1] The opto-electronic properties of these molecules can be influenced easily by p-extension and substituents.[1,2] Especially threefold substitution of HBCs indicates interesting changes in the absorption behavior, but only a few examples are reported.[2,3] A reason therefore could be the challenging synthetic access of suitable D_{3h} symmetric HBC building blocks.[2,4] Here, we present a new synthetic strategy for the synthesis of threefold iodinated HBC derivatives, which serve as ideal precursor to undergo further cross coupling reactions. First, the HBC moiety was substituted with electron acceptors *via* acetylene spacers to generate C_3 symmetric donor-acceptor compounds. Furthermore two/one electron acceptors and one/two electron donors (DAA/DDA systems) were coupled to the HBC core generating new asymmetric push-pull systems. The influence on the optoelectronic properties of the presented HBCs was analyzed by UV/Vis and fluorescence spectroscopy.



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Surface Chemistry of a (Sub-)monolayer [C_2C_1Im][OTf] Film on Pt(111): A Combined XPS, IRAS, and STM Study

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In a solid catalyst with ionic liquid layer (SCILL), ionic liquid coatings are used to modify noble metal catalysts to improve their selectivity. To understand the origins of this selectivity control, we performed model studies by surface science methods in ultrahigh vacuum. We investigated the growth and thermal stability of an ultrathin IL film by infrared reflection absorption spectroscopy and X-ray photoelectron spectroscopy in time-resolved and temperature-programmed experiments. We combined these spectroscopy experiments with scanning tunneling microscopy to obtain detailed insights into the orientation and adsorption geometry of the ions, and the wetting behavior in the first layer. Furthermore, we propose a mechanism for the thermal evolution of [C_2C_1Im][OTf] on Pt(111).

Extraction of hot carriers in colloidal $CsPbBr_3$ nanocrystals

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Extraction of hot charge carriers holds great promise for enhancing the solar energy conversion efficiency.[1] This study investigates the role of capping ligands in colloidal perovskites in facilitating the extraction of photogenerated hot electrons. By integrating colloidal $CsPbBr_3$ with fullerene-based capping ligands, we achieve efficient electron transfer with near-unity fluorescence quenching. The detailed hot carrier dynamics is studied by ultrafast transient absorption (TA) spectroscopy together with global analysis. Moreover, hot carrier cooling processes have been derived from the fitting of the high-energy tail of photoinduced bleach in TA spectra. We demonstrate the presence of fullerene ligands results in a three-fold increase in the relaxation time of hot carriers and a significant hot carrier extraction efficiency of 65.6%. This work underscores the potential of engineering surface ligands of colloidal perovskites to boost hot carrier extraction.

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Metalloenzymes in biological alkane oxidation

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Bacterial alkane oxidation is an efficient approach to functionalising the terminal C-H bond, which is a challenging reaction due to the inert nature of the bond. These bacteria can oxidise alkanes with high efficiency, specificity, and at ambient conditions. Most alkane oxidising systems comprise membrane-bound alkane monoxygenase (AlkB), a soluble Fe-S protein AlkG, and a reductase AlkT[1]. We are interested in studying the electron transfer processes involved in alkane oxidation pathways from unusual organisms, such as *Pseudomonas putida AlkG*, *Dietizia cinnamea* and *Polaromonas napthalenivorans.* Here, we present data of the characterisation of the two domain AlkG of *P.puitda*, C- and N-terminal regions. We have designed new constructs which involves a shorter C-terminal and a longer N-terminal domain. Affinity chromatography is used to isolate the protein of interest. Qualitative analysis is done by SDS-PAGE and EAS is used to characterise the 300-600 nm region which involves LMCT and is characteristic of these proteins. Later, these can be utilised to study the electron transfer pathway *in vitro* with Cyt C as a terminal electron acceptor.

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Modular Chemical Patterning of Graphene by Direct Laser Writing Using λ3 iodanes

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Covalently binding addends on graphene represents a viable option to address the challenge of the material's lacking band gap and is accompanied by additional benefits, such as fine-tuning its chemical properties by introducing functional moieties.[1] These functionalities augment the outstanding properties of graphene and can enable e.g. molecular recognition and catalysis.[2, 3] Precise control over addend binding to specific graphene surface regions extends the flexibility of the material and allows for the development of surfaces and devices tailored for specific demands. The emerging laser writing represents a promising strategy for covalent 2D patterning of graphene, yet remains a challenging task due to the lack of applicable reagents. Here, we present a versatile approach for the covalent laser patterning of graphene using trivalent iodine compounds as effective reagents, allowing for the engraving of a library of functionalities onto the graphene surface.

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Twisted Molecular Nanoribbons – Charge-Transfer Formation Competes with Singlet Fission via a Mixed Electronic State

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Nanoribbons (NRs) constitute a versatile platform for the development of novel materials. One approach to precisely generate NRs focuses on their bottom-up synthesis, i.e., the fusion of different types of functional components.[1] The specific composition of the resulting multichromophoric architectures not only determines their optical and electronic properties but also yields diverse excited-state dynamics. Here, we report on a set of twisted molecular NRs obtained by linear fusion of perylene diimide to pyrene and pyrazino- or thidiazolo-quinoxaline residues, endowing the NRs with electron donor-acceptor character. By employing various temperature-dependent spectroscopy techniques, we probed their complex excited-state interactions. The pre-twisted NR geometry favors the formation of a mixed electronic state.[2] Its fate is susceptible to polarity and rigidity of the environment as well as molecular geometry and length of the NRs. Efficient triplet generation is found in low-polarity solvents, whereas evidence for a (diabatic) charge-transfer state is gathered in solvents with higher polarity.

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Designing Discotic Amphiphilic Porphyrin-PAH Conjugates for Intramolecular Photoinduced Charge Separation

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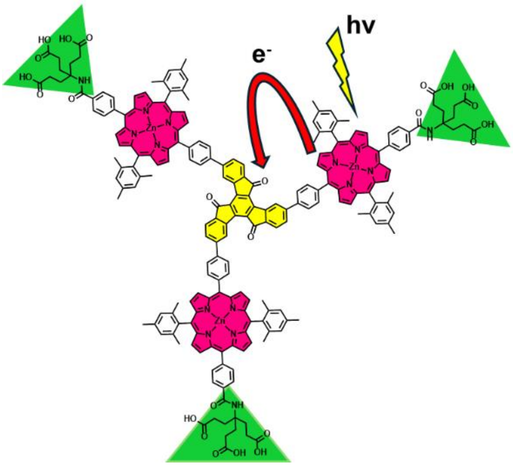
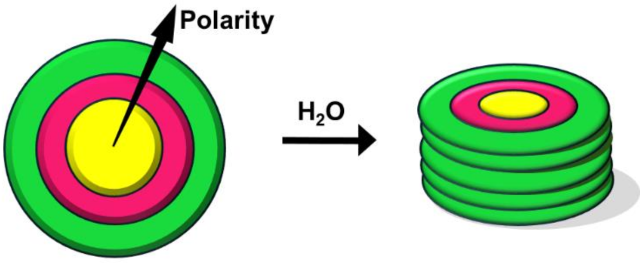
Porphyrins have already been used as efficient donor moieties in architectures with carbon-rich acceptor moieties such as fullerenes to generate photoinduced charge separation as well.[1] Here, we present the synthesis of novel discotic amphiphilic porphyrin-PAH conjugates, where a PAH is used as the central fragment, which is functionalized on its periphery with zinc-porphyrins. These in turn, possess Newkomb-dendrons to facilitate solubility in aqueous media. By using electron deficient PAHs such as truxenone derivatives or decacyclene triimide, a photoinduced charge separation from the porphyrin to the nonpolar, central PAH can be achieved. In aqueous solutions, these compounds are expected to form columnar stacks, due to the hydrophobic effect. The nonpolar interior of these stacks might be used as a reaction pocket for small nonpolar molecules, such as quinones, which could be reduced, mimicking the Q cycle in photosynthesis.





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Structural Insight into the Binding Mode of HDAC6 and its Inhibitors

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Post-translational modifications are *key mechanisms to increase proteomic diversity*. One of the post-translational modifications of histones is the reversible acetylation of lysines performed by histone acetylases (HATs) and histone deacetylases (HDACs). The enzyme HDAC6 can shuttle between the nucleus and the cytoplasm, giving it the ability to interact with histones but also with non-histone proteins. It is involved in cellular processes like cell signaling, inflammation, protein degradation, cell motility and cell survival. Overexpression of HDAC6 leads to imbalances in various cellular functions and is therefore associated with neurodegenerative diseases, cancer, and viral infections. [1] To counteract this overexpression, inhibitors have been developed, which currently lack efficiency and specificity. Using X-ray crystallography, we were able to solve high-resolution structures of HDAC6 in complex with two promising inhibitors. The structures allow us to gain insight into the binding mode of these highly active inhibitors to the enzyme and will facilitate the rational design of new HDAC6-specific inhibitors in the future.

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Excited state dynamics and performance optimization of diketopyrrolopyrrole-based DSSCs for solar energy conversion

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Three diketopyrrolopyrrole-based dyes were incorporated into DSSCs, featuring a layer of TiO_2 nanoparticles as semiconductor, iodide/triiodide redox electrolyte, and a platinum counter electrode. Optimization of these devices with respect to I_2 and Li^+ concentration of the electrolyte and the thickness of the TiO_2 layer revealed an optimum concentration of 0.1 M for both I_2 and Li^+. Interestingly, the optimal layer thickness varied between the different dyes. All samples were characterized in depth on the basis of J-V assays, IPCE, and electrochemical impedance spectroscopy. Furthermore, fs- and ns- transient absorption spectroscopy for TiO_2-based and Al_2O_3-based cells provided fundamental insights into the DSSC excited state dynamics.

Macroscopic heat release – Electrochemically triggered back-conversion of a molecular solar thermal system

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Molecular solar thermal (MOST) systems are photoswitches (photoisomers) that combine solar energy conversion, energy storage, and release in one simple molecular system.[1] One approach to release the stored energy is to use electrochemical triggers.[2,3] In this work, we monitored the electrochemically triggered heat release of the MOST system 3-cyano-3-(3.4-dimethoxyphenyl)norbornadiene/quadricyclane (NBD'/QC') macroscopically and analyzed the product composition by IR spectroscopy. We compare the macroscopic heat release with in-situ IR spectroscopic data and electrochemical characterization.

We demonstrate that we can trigger the heat release efficiently, switch off the reaction on demand, and control the reaction kinetics by the applied potential. As already small concentrations of the electrochemically formed $QC'^{+\cdot}$ are sufficient to catalyze the non-redox reaction from QC' to NBD', the additional energy input minimally avoids efficiency losses in the conversion cycle.

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Synthesis and Characterization of N-heterocyclic HBCs

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Hexa-*peri*-hexabenzocoronene (HBC), one of the smallest nanographenes, arouse high interest as promising candidate for possible applications in photovoltaics or organic electronics.[1] Introducing different substituents to the HBC's periphery provides an easy way to alter its properties, especially its optoelectronic characteristics. Herein, we report the influence of the substitution rate on the absorption and emission behavior of tri- and tetra-substituted N-heterocyclic HBCs.[2] In addition, the chosen benzoindole substituent was further fused to the HBC core *via* Scholl-type oxidation, to extend the p-system even more. Characterization of the molecules was achieved by NMR, MALDI-TOF mass spectrometry, UV/vis and fluorescence measurements.

Current work focuses on the synthesis of pyridinium HBCs with quaternized nitrogen directly bonded to the HBC core by utilizing S_N2 and Cu(II) mediated cross-coupling reactions.

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Norbornadiene, Bicyclooctadiene, Bicyclononadiene – Effects of a longer bridgehead on photoswitching and thermal back conversion

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Norbornadiene (NBD) is a molecule, which piques interest for molecular solar thermal energy storage (MOST). Through irradiation of light NBD derivatives undergo an intramolecular ring closure to form quadricyclane (QC).[1] The NBD/QC-system is well studied and recently theoretical calculation showed higher energy storage capabilities with increased lenght of the bridgehead.[2,3] Two of those systems are bicyclooctadiene (BOD)/tetracyclooctane (TCO) and bicyclononadiene (BND)/tetracyclononane (TCN) structures. While BOD/TCO and BND/TCN have higher differences in their ground-state energies, TCO and TCN suffer in regards of thermal stability. To understand the differences between those systems stationary and time resolved spectroscopic measurements were performed.

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Low Valent Iron Complexes Utilizing Variations of the TIMMN Ligand Framework

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The established TIMMN$^{\text{Mes}}$ ligand ***t**ris-[(3-mesityl**im**idazol-2-ylidene)**m**ethyl]ami**n**e* and the new adamantyl derivative were utilized to synthesize the corresponding iron complexes $[(\text{TIMMN}^{\text{R}})\text{Fe}^{\text{II}}(\text{Cl})]^{+}$ (**1**), $[\text{Fe}^{\text{I}}(\text{TIMMN}^{\text{Ad}})]^{+}$ (**2**) and $[(\text{TIMMN}^{\text{Mes}})\text{Fe}(\text{L})]^{+}$ (L = free site h^{1}-N_2, CO, py) (**3**) complexes. Complexes **1 – 3** demonstrate the notable steric and electronic flexibility of the TIMMN$^{\text{R}}$ framework by variation of the Fe–N anchor and Fe–carbene distances, as well as the variable size of the axial cavity. This is illustrated by the oxidation of $\mathbf{3^{Mes}\text{-}N_2}$ and **2** in a reaction with benzophenone to yield the corresponding, charge-separated Fe(II) radical complex $[(\text{TIMMN}^{\text{R}})\text{Fe}(\text{OCPh}_2)]^{+}$ (**4**). Further reduction of $\mathbf{3^{Mes}\text{-}N_2}$ leads to the Fe(0) complex $[(\text{TIMMN}^{\text{R}}\text{Fe}(\text{CO})_3]$ (**5**). In conclusion, the tris(carbene) chelate is not only capable of stabilizing the super-oxidized Fe(VI) and Fe(VII) nitrides but equally supports the iron ion in very low oxidation states, namely 0 and +1.

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Orthogonal Photoswitching in Solution and Photochromic Polymers with Application in Molecular Computing

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Gaining control over multiphotochromic systems is of great desire. By combining two indigoid photochromes, a rhodanine-based photoswitch and a *peri*-anthracenethioindigo (PAT), a highly controllable system with all-visible light, all-photon, path-independent and fully orthogonal photoswitching is established. All four possible states are light-induced addressable resulting in high isomeric yields using only non-toxic visible light. Independent from the starting state and irradiation sequence all states can be selectively populated. The four states can be distinguished either spectrally or by their color with the naked eye which makes it possible to transfer the concept to polymers. Embedding the two photoswitches into a solid polymer matrix a multiphotochromic material is developed that changes its color upon irradiation with light. By combining the orthogonal photoswitching system with a fluorophore complexity is even increased enabling application as all-photonic molecular logic gates and molecular encoders.

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Extended coherent electron accelerator on a nano-photonic chip

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Today's classical particle accelerators use radio-frequency metal cavities to accelerate and confine particles by synchronizing a microwave travelling wave with the particle propagation. We have shown the same principle, but in the optical domain and with dielectric materials. With advances in laser and nanofabrication technology the miniaturization of such devices is possible. This talk will cover the acceleration of electrons from 28.4 to 40.7 keV in a 500 µm long structure. Not only do we accelerate the electrons, but we also confine them with the help of the optical fields transversely utilising the alternating phase focussing scheme. This way, we can accelerate the electrons inside of a 250 nm narrow channel [1]. This could lead to a new type of accelerator that fits on a chip for applications in science, medicine, and industry.

Ion-electroadsorption devices based on electrical double layer capacitors (EDLCs) present a new avenue for energy efficient ion-based computing. Especially, capacitive analogues of semiconductor-based diodes (CAPodes) with high rectification ratio are attractive for a great number of technological applications, such as logic gates. High rectification ratios render CAPodes attractive for a great number of technological applications, from energy storage to alternating current (AC) rectification and logic gates. Here, we disclose the general concepts for bias-direction-adjustable n- and p-CAPodes achieved by selective ion sieving. Controllable-unidirectional ion flux is realized by blocking electrolyte ions from entering sub-nanometer pores, leading to an efficient sieving effect at pore size below the size of bulky cations or anions. A precise regulation concept can effectively balance the current between positive and negative bias. The resulting CAPodes exhibit charge-storage characteristics with a high rectification ratio (RR_{II}, 96.29%). The enhancement of capacitance is attributed to the high surface area and porosity for our proposed omnisorbing carbon, leading to a larger ion-accessible pore space that enables rapid charge storage kinetics. Furthermore, we demonstrate the use of an integrated device in a logic gate circuit architecture to implement 'OR' logic operations. This work demonstrates CAPodes as a generalized concept to achieve p-n and n-p analogue junctions based on selective ion electrosorption, illustrates the enormous diversity and complexity attainable in CAPode systems, provides a comprehensive understanding and highlights applications of ion-based diodes in ionologic architectures.

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Pushing the Limits Towards Long-Lived Charge Separation in Ruthenium (II) Phthalocyanine-Subporphyrazine Conjugates

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In the context of solar energy conversion research, electron donor-acceptor (D-A) systems have gained interest for their ability to produce long-lived charge-separated states, convertible into useful forms of energy upon photon capture. Porphyrinoids, particularly phthalocyanines, are frequently chosen as chromophores in D-A arrays owing to their tunable optoelectronic properties and rapid energy/electron transfer capabilities.[1] Ruthenium(II) phthalocyanines (RuPcs) have been widely incorporated in D-A systems as they afford stable and strongly coordinated assemblies, promote rapid charge separation, and feature slow charge recombination.[2] Subporphyrazines (SubPzs), a class of contracted porphyrinoids, exhibit outstanding optoelectronic properties that can be tailored through functionalizations.[3] RuPcs, combined with SubPzs, cover a wide range of solar radiation spectra, absorbing between 250 and 700 nm. Here, we present a series of RuPc-SubPz conjugates, which display energy and electron transfer reactions depending on SubPz structural design, showcasing their potential for advancing the efficiency of artificial photosynthetic systems.

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Spatially resolved 2D Laser Writing of Graphene with Diazonium Salts

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Modifying graphene via covalent functionalization by introducing various functional moieties and therefore tuning the chemical properties has established itself as a key field in graphene research.[1] Modern 2D patterning techniques, which combine highly efficient, covalent functionalization with precise spatial resolution, allows a dimensional and quantitative control over the addend binding.[2] Herein, we present an optimized protocol for the laser-activated spatially resolved functionalization of graphene using various diazonium salts exhibiting different functional groups, where the laser writing behavior of 4-*tert*-butylbenzenediazonium tetrafluoroborate (**4-TBBD**) is presented in detail.

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Combining 3D Printing and promising Electrolyte Research: Ionic Liquid based Membrane Materials

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As promising components in energy devices such as fuel cells and batteries ionic liquids (ILs) are discussed due to their favorable properties. These salts with melting points below 100 °C show e.g., high thermal and electrochemical stability, high ionic conductivities and non-flammability, making them interesting candidates for use as electrolytes. [1] Therefore, ILs can play an integral part in the advancement of energy technologies that are so vital for the necessary energy transition.

The aim of this work is the synthesis and characterization of ILs for proton conduction. The ILs exhibit wide electrochemical and thermal stability windows and high ionic conductivities at elevated temperatures. Moreover, the ILs are immobilized in different polymers to provide ionogels that show promising electrolyte properties after addition of the ILs. Successful 3D-printing of the IGs is also demonstrated. [2,3]

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Enhanced Internal Electric Field of CdS/NU-M Z-Scheme Heterojunction for Efficient Photocatalytic Hydrogen Evolution

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Photocatalytic hydrogen evolution offers solutions to the energy crisis and environmental pollution. Metal-organic frameworks (MOFs) as high-efficiency photocatalysts often face challenges in charge separation and transfer. We developed a cadmium sulfide/zirconium-based metal-organic framework (CdS/NU-M) heterostructure using 4-mercaptobenzoic acid (4-MBA) for interfacial linker coordination. This reduced the energy difference between the conduction band of NU-M and the valence band of CdS, creating an enhanced internal electric field and efficient charge separation via a Z-scheme mechanism. The CdS/NU-M achieved a hydrogen evolution rate of 84.3 mmol g^{-1} h^{-1}, surpassing many MOFs and CdS-based photocatalysts. This study highlights the crucial role of interfacial linker coordination in enhancing charge separation and transfer, thereby significantly improving photocatalytic performance.

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Non-covalently functionalized cobalt-phthalocyanine transition metal dichalcogenide nanosheet networks

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Solution-processed nanosheet networks (NN) of exfoliated transition metal dichalcogenides (TMDs) have attracted immense interest which is partially attributed to their compatibility with printing techniques, suitable for large area processing. The electrical characteristics of the NN obtained from liquid–liquid interface deposition, demonstrate an electron mobility of 10 cm^{2}V^{-1}s^{-1} for networks of molybdenum disulfide nanosheets [1].

The TMD NN's semiconducting nature offers opportunities for adjusting electronic properties through functionalization, especially with thiopyridyl-cobalt phthalocyanines (CoPcs). These molecular building blocks have previously demonstrated effectiveness in carbon capture mechanisms. [2].

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Integrating AI in Automated Lab Methods for Enhanced Generation and Analysis of *In-Vitro* 3D Human Tissue Models

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Developing *in-vitro* tumor tissue models is essential for personalized cancer treatment. These models enable the study of tumor biology and drug effects, providing valuable insights for therapeutic strategies. However, manually analyzing morphological changes from drug treatments is labor-intensive and prone to inaccuracies, requiring quantification to refine therapies and improve drug screening. To address these challenges, integrating AI into automated lab methods can standardize and streamline the generation and analysis of tissue models. While automated systems have improved efficiency in various fields, their use in life sciences often focuses on specific steps rather than entire procedures.

This study, demonstrates the integration of AI to both the robot-assisted production and analysis of three-dimensional tumor tissue models. Methods are employed to monitor and guide automated production and analyze the resulting tissue models. Four key applications are demonstrated: cell identification and counting, monitoring pipette tip un-packaging, detecting cell culture plate positions, and characterizing spheroidal tumor tissue models. This AI-supported approach enhances efficiency and accuracy, paving the way for more advanced and reliable research methodologies.

Antimicrobial photodynamic activity of chlorophyllin against *Pseudomonas aeruginosa*

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Pseudomonas aeruginosa persister cells are slow-growing sub-populations that significantly contribute to antibiotic tolerance and recalcitrance of infections, presenting a notable medical challenge. Currently, little is known about the photodynamic inactivation of persister cells. Here, we investigate the influence of the photosensitizer chlorophyllin (CHL) exposed to red LEDs alone and in combination with the cationic permeabilizer polyethylenimine (PEI) or the activator of mechanosensitive channels butylparaben (BP) on *P. aeruginosa*. Antimicrobial susceptibility tests were performed using the broth microdilution checkerboard method. Serine hydroxamate was used for the induction of persister cells via amino acid starvation. Interestingly, persister cells exhibited more sensitivity to CHL/PEI combinations compared to growing cells [1]; whereas they were less sensitive to CHL/BP combinations. Our findings demonstrated the synergism between illuminated CHL and PEI or BP against *P. aeruginosa* growing and persister cells with exposure times of 60 min or less. These findings suggest the potential of these combinations for combating *P. aeruginosa*.

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Mechanistic Insights of Tunable Iridium(III) Complexes as Sensitizers for Organic Photocatalysis *via* Triplet-triplet Energy Transfer

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Photosensitization has proven to be a valuable method in the synthesis of (newly developed) organic molecules, improving (enantio-)selectivity, functional group tolerance as well as lowering costs and limiting safety concerns. A valuable mechanism in the photosensitization process has been triplet-triplet energy transfer (TTEnT) catalysis, which circumvents harsh UV-light irradiation.[1] For an effective energy transfer towards different reagent molecules, tunable photosensitizers are eminent. Cyclometalated Ir(III) complexes have shown to be not only tunable, but also efficient triplet-triplet energy transferring photosensitizers.[2] Combining these complexes with a two-dimensional reaction- and mechanism-based screening approach, we achieved various novel synthesis routes. Though, the mechanism of the photocatalysis can be very complicated and is therefore under continuous investigation. We provide new insights in these mechanisms, elucidate emerging equilibria and eliminate unwanted reaction pathways.

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Tunning the Twist by Molecular Design: A New Strategy for Pyrene-Containing Helical Twistacene

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The study of atomically precise nanographenes (NGs) is crucial to fully exploit their potential applications since their properties are highly dependent on structural variables. However, the synthesis of extended NGs is a current challenge as it requires the generation of soluble and stable intermediates, which makes purification, characterization, and processing difficult, thereby limiting the comprehensive exploration of their fundamental properties. Consequently, improvements in the design of these systems appear crucial to overcome such a limitation. In this work, we present the synthesis of a helical-twisted hexacene, which exhibits an end-to-end torsion angle value of approximately 145º. The synthetic strategy involves a sequence of two Diels-Alder cycloadditions based on aryne chemistry.[1] In addition, the high solubility in organic solvents at room temperature allowed their purification by chromatographic methods, followed by a complete structural, optoelectronic, and electrochemical characterization.

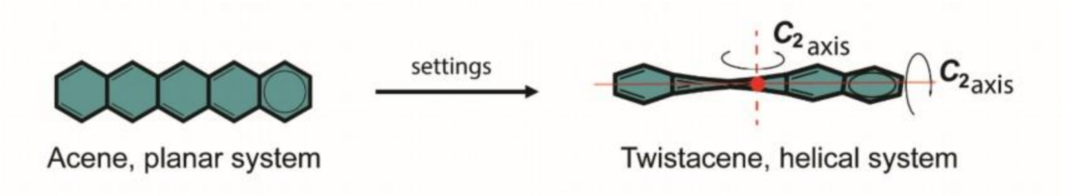

Figure 1*.Schematic representation of helical-twisted hexacene.*

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Synthesis & Chiro-optical Properties of a Nanographene-embedded Conjugated Macrocycle

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Macrocyclic hydrocarbon nanostructures have recently attracted a lot attention due to their optoelectronic properties and their possible use as supramolecular receptor with application in numerous fields such as catalysis or selective purification. In this work, we report the synthesis of a new type of chiral macrocycle incorporating curved heptagon-containing extended PAH unit and a helicene embedded. The photophysical and electrochemical properties were investigated by UV–vis absorption and fluorescence spectroscopy as well as by cyclic and square wave voltammetry. Moreover, the two enantiomers **(*M*)/(*P*)-1**, were successfully resolved and isolated by HPLC and studied by CD and CPL spectra. The novel macrocycle can act as supramolecular receptor of curved π-systems based on concave convex complementarity.[1] This proof-of- concept system shows that saddle-shaped PAHs play an important role in the design of new host, with potential applications in chiral recognition.

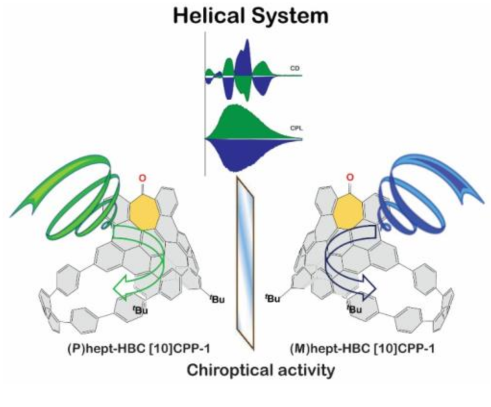

Figure 2. *Schematic representation of* **(*P*)/(*M*)-1**

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2D-Engineering of Graphene – Parameter Study for the Laser Triggered Covalent Functionalization

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Covalent functionalization of graphene is a powerful tool to tune the materials unique properties. The development of various methods to achieve locally controlled modifications was a tremendous step towards tailor-made graphene based materials. Herein, we present a fundamental study regarding the laser activated spatially resolved functionalization of graphene using dibenzoyl peroxides as model compounds with an unprecedented level of control in terms of the degree of functionalization, the lateral resolution and the attachment of different functional moieties in an iterative process. We also present two pathways to prove the reversibility of the functionalization in a large scale and a locally controlled manner, offering a full write – read – store – erase sequence.

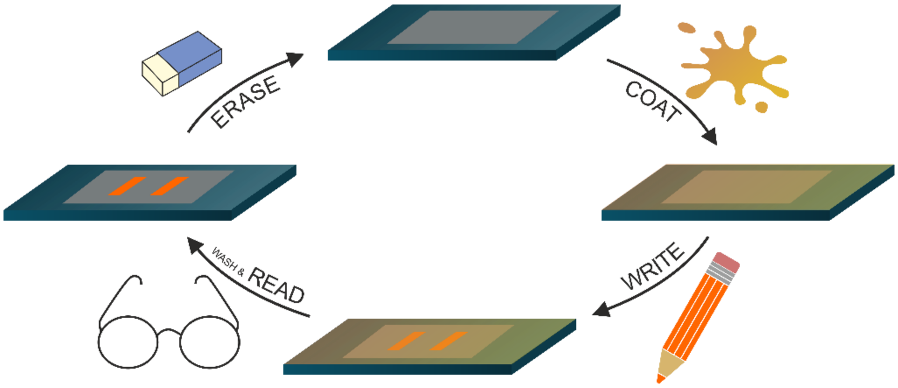

Figure 1. Schematic representation of the coat - write – read – erase cycle.

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Photoconductive Perylenebisimide Cyclophane-Fullerene Hybrids

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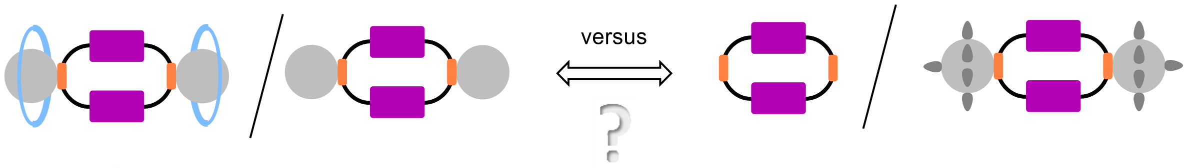
Despite the huge attention that fullerenes have attracted as electron acceptor molecules in organic electronics and photovoltaics, fullerene derivatives tend to aggregate, which causes low efficiency of photocurrent generation. Perylenebisimide based cyclophanes have been used as architecture to prepare dumbbell molecules bearing two C_{60} substituents and their corresponding supramolecular pseudo-bisrotaxane with [10]cycloparaphenylene,[1] which should overcome the problem. Their photoconductive behaviour in terms of photocurrent generation and photopotential have been addressed and compared to those of the parent cyclophane as well as to a functionalized fullerene-cyclophane dumbell molecule, which should be photochemically inactive (Figure 1).[2] The role of the fullerene substitution both covalently and supramolecularly have been investigated.



$([10]CPP)_2{\supset}P2(C_{60})_2$ **$P2(C_{60})_2$** **P2** **$P2F2_{C18}$**

Figure 1. Schematic representation of the photoconductive molecules

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Synthesis and Characterization of a Helical-Twisted Nanographene

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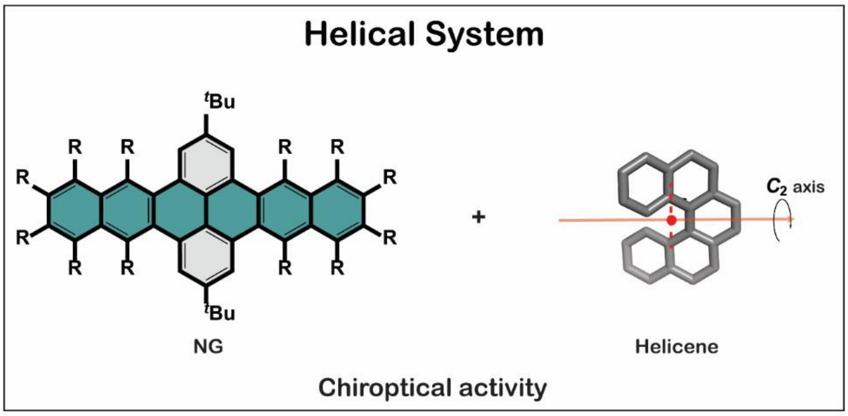
Organic solar cells have the potential to revolutionize renewable and sustainable energy, but we must drastically improve the conversion efficiency. Singlet Fission "SF" has emerged as a promising strategy to boost their performance by avoiding the loss of extra energy by thermalization in solar cells.[1] SF has been observed in various families of polycyclic aromatic hydrocarbons (PAHs), among which the acene family has shown a prominent position, with triplet quantum yields (TQY) exceeding 200% for pentacene.[2]

Additionally, the introduction of helicene in PAHs [3] produce the emergence of new properties, such as chirality, which have significant applications in nonlinear optics. To address this, we are designing new chiral NG with improved solubility, high stability and promising properties for SF.

Figure 3 Schematic representation of helical system.



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Synthesis and Investigation of Norboradiene-Perylenediimide Dyads towards Molecular Solar Thermal System Application:

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Today's population is facing a massive gap between the worldwide demand for energy and the currently insufficient supply of non-fossil fuel-based energy sources.[1] One approach for emission-free energy capturing are molecular solar thermal energy storage (MOST) systems like the strongly researched norbornadiene-quadricyclane (NBD/QC) interconversion couple. Its photophysical properties can be finely tuned by coupling to perylene-diimide (PDI) cores which results in intriguing absorption and interconversion behavior.[2] By attaching the NBD/QC couple to the PDI core at different positions and by variable linkers, interesting alternations of the system's photophysical properties are observed.

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Oxidation of acetol with earth abundant metal salts

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In recent years, oxidation reactions have evolved from toxic Cr(VI) chemistry towards various TEMPO mediated syntheses [1]. To go a step further towards green chemistry we aim for earth abundant metals to catalyze the oxidation of the α-hydroxy ketone acetol to its corresponding acid as a model reaction applying green chemistry principles.
For this purpose, we chose Mn(II), Ni(II), Co(II), Cu(II) and Fe(III) salts as homogeneous catalysts in aqueous solutions and strong oxidants like H_2O_2, that produce rather harmless waste. The variation of all relevant reaction parameters, such as temperature, pH-value and concentration of all included substances, but also the process design, is crucial to find the optimal reaction conditions for a high selectivity.
Currently, the product spectrum consists of different oxidation products like lactic acid, acetic acid, formic acid and the desired product pyruvic acid. The highest conversion was observed in a system with $FeCl_3$. However, the best results regarding selectivity were achieved using $CuCl_2$.

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In situ monitoring of molecular sieve synthesis via ultrasonic attenuation

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Molecular sieves, viz. zeolites and metal organic frameworks, are crystalline, microporous structures with a three-dimensional framework. Due to their high surface area, molecular sieves are used as adsorbents and as catalysts in exhaust gas treatment [1].

Understanding the synthesis of these materials remains a challenging task. Various mechanism models for the formation have been proposed [2, 3]. The in situ monitoring with ultrasonic attenuation is a non-destructive method, with a high time resolution providing new information about the mechanism of molecular sieve synthesis.

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Implementation of an in situ atomic force microscope (AFM) setup to study the dynamics of (electro-)catalytic interfaces

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Electrochemical atomic layer deposition (EC-ALD) is a promising technique for precise and controlled deposition of thin films on surfaces. ALD requires self-limiting reactions, which can be done by underpotential deposition (UPD). In UPD, up to a monolayer of a metal is deposited on a substrate at a potential that is more positive than its thermodynamic deposition potential.[1] To better understand EC-ALD processes, we need to understand the morphological changes of the thin film formation at the molecular/atomistic level.

High-resolution atomic force microscopy (AFM) can provide the required information. We implemented a new in situ AFM setup (Cypher AFM, Oxford Instruments), which permits studies under reaction conditions at gas/solid, liquid/solid, and electrochemical interfaces. In particular, the in situ cells allow us to precisely control the experimental parameters such as temperature, pressure, and flow rates of gases and liquids, and the applied potential. Thus, we can study the formation of thin films by EC-ALD in situ by high resolution AFM.

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Characterization of Novel Carbon-Rich Architectures by First-Principles Calculations

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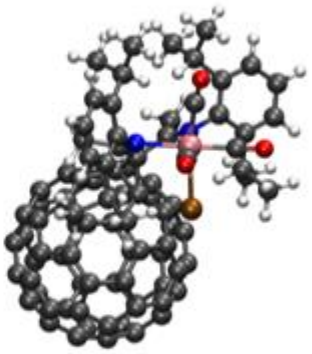
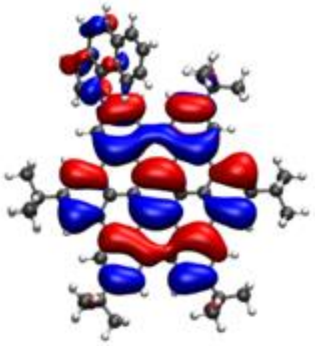
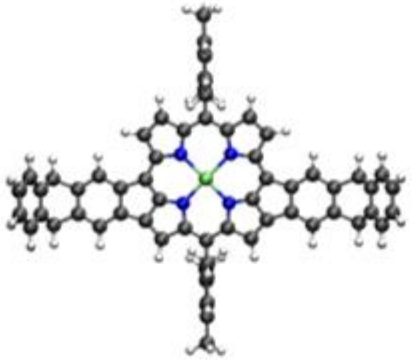
Atomistic quantum-chemical calculations have become an integral part of many studies in organic, inorganic and physical chemistry. Theoretical support ranges from simple structure optimizations and energy calculations for analyzing thermodynamic stability, to providing spectroscopic fingerprints, e.g. IR or UV-Vis spectra, to extensive studies clarifying reaction pathways. Calculations can provide complementary data, which can be essential for the interpretation of experimental observations.

Here we present a series of collaborations where these joint efforts between experiment and theory are exemplified. Density-functional theory (DFT) was used to clarify the geometry of different fused porphyrin conjugates, their orbitals and energies. Using the nudged elastic band (NEB) method, possible pathways and activation barriers for rotation of substituents bound to an HBC core are explored and compared to experimental observations. In addition, time-dependent DFT is used for calculating UV-VIS absorption spectra to confirm the exact conformation of reaction products. Finally, different binding sites of triptycene–porphyrin structures and their ability to catch and bind fullerenes are analyzed and compared to mass spectrometry results.







Reversible C═N Bond Formation Controls Charge-Separation in an Aza-Diarylethene Photoswitch

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Diarylethenes are one of the most prominent photoswitches that have been highly optimized over the last decades. Due to their strong photochromism, thermal stabilities and fatigue resistances, they are found in many material and biological applications that need precise control of states. In this work, we present the first pyrimidine-based aza-diarylethene four-state multi-stimuli photoswitch, that undergoes a reversible zwitterion-forming photoreaction. In this process, a C=N bond is generated under concomitant formation of a positively charged aromatic pyrimidinium moiety under consecutive formation of a conjugated, negatively charged thiolate group. The zwitterion shows negative solvatochromism in apolar solvents bridging the properties of merocyanines and diarylethenes. Upon protonation, the thiolate group can further undergoe a photo-induced double bond isomerization between the preorganized *Z* isomer and its *E* isomer. Therefore, acid addition not only enhances the addressability of states, but modulates thermal isomerization barriers from a highly dissipative system, to a highly stable one, again in a fully reversible fashion.[1]

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Hexabenzocoronene meets Porphyrin: A Fusion Enabling the Modification of Excited-State Lifetimes from µm to ps!

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The great significance of porphyrinoids in the fields of photophysical and biological application resulted in extensive research in the last century.[1,2] Especially for the application in photovoltaic application the moderate absorption in the near-infrared (nIR) is a limiting factor.[3] In order to tackle this drawback the expansion of the porphyrin core at the *β*- and *meso*-positions has emerged as an effective strategy.[4,5] Here, we report in the characterization of five porphyrin dyes fused via a 5-membered ring to HBC (**2HFP1**, **2HFP2**, **2HFP3**) and benzene (**2HFP4**, **2HPF5**), respectively. The resulting absorption features of these molecules are of interdisciplinary interest in the fields of organic photovoltaics and nIR dyes. Additionally, HOMA calculations suggest that the newly formed 5-membered rings induce biradicaloid character into the pyrrole ring of the porphyrin. This strongly impacts the excited state lifetimes. Confirmation for this was obtained by time-resolved transient absorption measurements. Here, broadened absorption characteristics as well as short-lived excited states, with up to six orders of magnitude faster decay rates, are present in the spectra.

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Perylenebisimide – Porphyrin Architectures in Water

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An efficient way to address the challenge of tailoring the supramolecular assembly of donor-acceptor (D-A) systems lies in the utilization of the hydrophobic effect by the synthesis of integrated amphiphiles, consisting of suitable D-A couples, which has already been showcased in exemplary systems.[1,2] Architectures built from porphyrins and perylenebisimides (PBIs) are well-understood D-A systems and inherit remarkable properties,[3] but still, to this day, amphiphilic derivatives based on these couples are only sparsely explored.[4] Here, we report various architectures based on these chromophores, from bola-amphiphilic triads, discotic pentads, and hierarchical supramolecular assemblies.

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Investigating the QC-to-NBD back-conversion with Norbornadiene-Perylenediimide Hybrids

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Since energy storage with renewable resources is a challenge yet to be solved, scientists across the world are investigating molecular solar thermal (MOST) systems. A promising example is the photoinduced [2+2] conversion of norbornadiene (NBD) to the higher energy isomer quadricyclane (QC).[1] Current research is aimed at improving the system for real-world application by both tuning the photophysical properties of the NBD as well as developing catalysts for selective energy release.[2] Due to the highly electron-accepting nature and ability to form one electron reduced species upon photoirradiation, rylene diimides became of interest for the back-conversion of QC to NBD. Based on promising results with naphthalenediimides (NDIs)[3] and the larger perylenediimides (PDIs),[4] we investigated further NBD-PDI conjugates to study the effect of the linker on the back-isomerization.

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PM4Onco: Enhancing Personalized Oncology Through Integrated Clinical and Biomedical Data

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The joint project Personalized Medicine for Oncology (PM4Onco) initiated in 2023 as part of the National Decade Against Cancer, aims to establish a sustainable infrastructure for integrating clinical and biomedical research data within the Medical Informatics Initiative (MII). Combining expertise from all four MII consortia and leading German oncology centers, PM4Onco supports decision-making in Molecular Tumor Boards by preparing data to enhance targeted therapies. The project extends to 23 partner sites, improving access to treatments based on clinical information and molecular genetic analysis of tumors. Involving clinical cancer registries to standardize documentation and enhance data quality, PM4Onco also integrates patient-reported outcomes on quality of life and treatment efficacy. Patient representatives ensure that patient perspectives guide decision-making. By fostering collaboration among clinical experts, bioinformaticians, and patient advocates, PM4Onco aims to advance personalized medicine in oncology, improving treatment and prognosis for cancer patients. Initial results on data flows and requirements analyses are available. [1], [2]

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Solid-state NMR spectroscopic investigation of supported ionic liquids for catalytic applications

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Supported Ionic Liquid Phase (SILP) catalysts are promising materials with advantages for homogeneous catalysis, thanks to their ease of separation from the reaction media, its reuse potential, and the high tunability of its catalytic performance. SILP catalysts are obtained by impregnating a support with a mixture of an ionic liquid (IL) and a molecular catalyst. [1]

Solid-state nuclear magnetic resonance (NMR) spectroscopy is a suitable method for studying these materials. Here, we show how techniques like Cross Polarization (CP), REDOR, two-dimensional heteronuclear and homonuclear correlations, and ^{129}Xe NMR spectroscopy are crucial to gain detailed microscopic, even molecular understanding of the interactions within the IL film, the support material, and the solid-liquid interface.[2,3] Such knowledge is essential to fully exploit the potential of SILPs.

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Novel Norbornadiene/Quadricyclane Interconversion Couples as Potential Candidates for Molecular Solar Thermal Applications

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Among renewable energy sources, especially solar energy possesses great potential.[1] Regarding the conversion and storage of solar energy, one interesting approach is the use of so called molecular solar thermal (MOST) systems. One candidate considered for MOST applications is the norbornadiene/quadricyclane (NBD/QC) interconversion couple.[2] The photophysical properties of the NBD/QC system can be fine-tuned by attaching various functional groups to the to the norbornadiene core. For example, a so called "push-pull" system can be created by attaching electron donating and electron withdrawing groups to one double bond, resulting in a bathochromic shift of the absorption maximum.[3] The here presented library of "push-pull" NBD derivatives were investigated regarding their photophysical properties using NMR und UV/Vis spectroscopy as the main characterization methods.

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Missing Plants: Difficulties in Recovering Lipid Plant Signatures from Experimentally Produced Pottery Residues

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Lipids absorbed into archaeological pottery can reveal foods eaten by ancient societies, but often reveal mostly animal-derived resources. Many plant-based foods remain underreported or undetectable in archaeological pottery residues, due to their lower lipid content. The goal of our research is to address these gaps in knowledge by improving the detection of plants in pottery residues. We conducted a multi-commodity cooking experiment to locate potential biomarkers of foodstuffs thought to have been important to Roman Britain, as part of the Roman Melting Pots project. Repeated cooking episodes with eight plant and plant-derived commodities were conducted to produce residues in replica Roman cookware. Extracted residues were analyzed by liquid and gas chromatography coupled with high-resolution mass spectrometry [LC-HRMS,GC-HRMS] and compared to the lipid signatures of raw food correlates. It is clear that a complex relationship exists between lipid absorption and cooking practice. This experimental research shows the challenges of identifying plant residues even in highly controlled laboratory conditions. Main challenges will be discussed and their implications for archaeological lipid residue research.

Archaeal Tetraether Lipids for Improved Stability and Application of mRNA Vaccines

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The tetraether lipid GDGT (glycerol dialkyl glycerol tetraether) from Archaea is exceptionally stable due to its ether linkages and cyclic alkyl chains, making it ideal for forming archaeosomes that withstand extreme conditions regarding acidic pH values and temperature. This study investigates GDGT archaeosomes as an oral delivery system for mRNA vaccines, aiming to improve patient compliance, hygiene, and cold-chain storage.

Different formulation techniques were compared regarding size, polydispersity and charge, and optimized via Design of Experiment. The incorporation of mRNA was optimized by varying lipid compositions and nitrogen/phosphate ratios. Optimized archaeosomes, around 100 nm in size with a zeta potential of –30 mV, showed high stability and mRNA protection in acidic gastric conditions.

These GDGT-based mRNA archaeosomes demonstrated superior transfection rates in CHO-K1 cells under serum conditions compared to the standard lipofectamine, using enhanced green fluorescent protein. Thus, GDGT forms stable, nano-sized archaeosomes with promising applications in oral mRNA delivery.

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Host-Guest Complexes of Dibenzopentalene-Containing Cycloparaphenylenes in Mass Spectrometry

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Cycloparaphenylenes (CPPs) are conjugated molecules consisting solely of sp^2 hybridized carbon atoms. Due to their concave and convex π arrays, CPPs excel as supramolecular hosts for fullerenes [1] and CPPs [2].

This study focuses on diketo- and tolyl-substituted dibenzopentalene-incorporated CPPs (DBP-CPPs) as hosts for C_{60}/C_{70} and [n]CPPs. Analysis via electrospray ionization mass spectrometry revealed [1:1] complexes formed between DBP-CPPs and C_{60}/C_{70}, and [6-8]CPPs. Energy-resolved collision (MS^2) experiments show that DBP-CPP$\supset$fullerene [1:1] complexes are less stable than their CPP counterparts due to higher strain energy from the DBP unit. Singly charged DBP-CPP$\supset C_{70}$ complexes show greater stabilities than C_{60} complexes, mirroring CPP behavior [2]. For [6-8]CPPs, complex stability decreases with increasing guest size. Notably, tolyl-DBP-CPP forms doubly charged complexes with [6]CPP, displaying charge separation absent in CPP$\supset$CPP complexes.

Our results highlight DBP-CPPs' potential as hosts for fullerenes and CPPs, with mass spectrometry proving powerful for probing these non-covalent complexes.

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