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Foreword

As members of the Women in Science-Erlangen Symposium Organizing Committee, it gives us immense pleasure to welcome you to the 4th edition of our symposium series at the Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg in Germany.

The Women in Science - 4th 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 inspiring young scientists.

We are delighted to welcome almost 200 participants from many different career stages to the 4th edition of our Symposium. Over the course of three days, top-notch female scientists from diverse research fields such as physical chemistry, computational chemistry, life sciences, and biology, among many others, will not only deliver their research findings, but they will also showcase their professional careers and personal experiences in academia and/or industry. All participants, from early-stage bachelor students to senior professors, will have the opportunity to establish new network connections and collaborations.

The symposium program includes invited lectures and flash talks, as well as poster and brain-dating sessions. In addition, considerable time will be devoted to discussing diversity and inclusion in the workplace, positive discrimination, and other relevant topics 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 participant to actively take part in the symposium.

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

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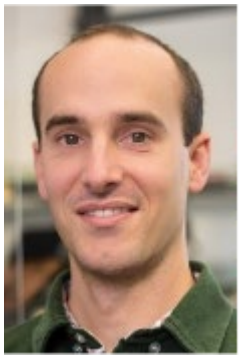

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Funding

The members of the Organizing Committee of WIS25 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 Wiley – Chemistry Europe for providing poster and flash talk prizes for our symposium.

Supporting research consortia at FAU

We are thankfull for the support of the following research consortia at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), funded by the **German Science Foundation** (DFG), through their means for promoting equality, with organizational support from **F^{3}G network** at FAU. Participating consortia are:

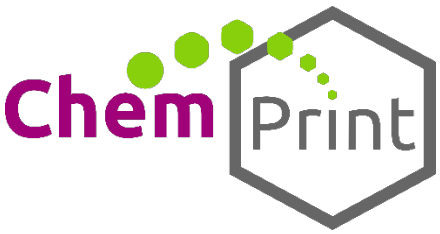
- CRC 1411 – Design of Particulate Products
- CRC 1540 – Exploring Brain Mechanics (EBM)
- CRC 1719 – Next-generation printed semiconductors (ChemPrint)
- RTG 2423 – Fracture across Scales (FRASCAL)
- RTG 2495 – Energy Conversion Systems: From Materials to Devices
- RTG 2861 – Planar Carbon Lattices (PCL)
- RTG 2950 – Solidification cracks during laser beam welding

Supporting institutions at FAU:

- Graduate School in Advanced Optical Technologies (SAOT)
- FAU Competence Center Engineering of Advanced Materials (FAU EAM)
- FAU Womens Representatives
- Department Chemistry and Pharmacy, FAU

Support from outside FAU:

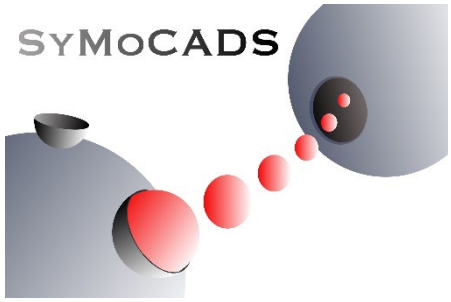
- FOR 5499 – Molecular Solar Energy Management Chemistry of MOST systems (FOR MOST)
- JungesChemieForum (JCF)
- Wiley – Chemistry Europe



ENGINEERING OF ADVANCED MATERIALS
FAU COMPETENCE CENTER

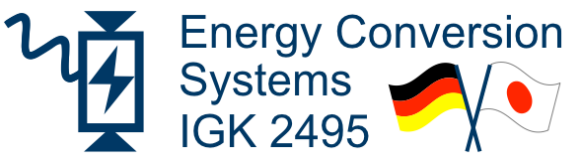
Chemistry A European Journal

Chem Bio Chem



ADVANCED THERAPEUTICS

Chemistry Europe



General Information

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

Photo: Staatliches Bauamt Erlangen-Nürnberg

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

Transportation

Airports:

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

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

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

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

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

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

Detailed Programme

	Wednesday	
	9:00 - 10:00	**Registration**
	10:00 - 10:30	**Welcome Speech (Ingrid Span)**
Session 1: Danijela Gregurec	10:30 - 11:10	**Stefanie Klein** *Magnetoplasmonic Nanoparticles for X-Ray triggered cancer therapy*
	11:10 - 11:20	**Flash Talk: Christina Müdsam** *With my feet in the air and my head on the ground*
	11:20 - 12:00	**Müge Kasanmascheff** *Unraveling Metalloenzymes:* *Insights from Advanced EPR Spectroscopy*
	12:00 - 13:00	**Lunch Break**
Session 2: Julien Bachmann	13:00 - 13:40	**Helen Hölzel** *Energy Management of Functional Molecular Materials*
	13:40 - 14:20	**Malika Jeffries-El** *Design and Synthesis of Organic Electronic Materials*
	14:20 - 15:00	**Ilka Paulus** *On the other side of the proposal*
	15:00 - 15:30	**Coffee Break**
Session 3: Siow Woon Ng	15:30 - 16:10	**Martina Preiner** *Energy Management of Functional Molecular Materials*
	16:10 - 16:20	**Flash Talk: Reyana Ganguly** *Structural and spectroscopic characterisation of AlkB domains involved in electron transfer during alkane oxidation*
	16:20 - 17:00	**Jennifer Munkert** *Bridging Two Worlds - An Academic Journey between Research and Teaching*
	19:00	**Speakers' Dinner (upon invitation)**

Thursday

Session 4: Müge Kasanmascheff	9:00 - 9:40	**Ani Özcelik** *Chasing Dreams with a Little (Chiral) Twist*
	9:40 - 10:20	**Anastasia Hager** *Expanding the Druggable Space – My scientific journey through the rapidly evolving world of pharmaceutical research*
	10:20 - 10:50	**Coffee Break**
Session 5: Ingrid Span	10:50 - 11:30	**Laura Dassama** *Chemical bioogy for human health*
	11:30 - 11:40	**Flash Talk: Ecem Aydan Alkan** *Tuning the Transparency and Exciton Transition of D-π-A-π-D Type Small Molecules*
	11:40 - 12:20	**Joanna Jankowska** *Computational (photo)chemist at work: Is there only one way to do it right?*
	12:20 - 13:30	**Lunch Break**
Session 6: Carolin Müller	13:30 - 14:10	**Lisa Pecher** *Chemical Connections Between People:* *A Place for the Authentic You*
	14:10 - 14:20	**Flash Talk: Anabel Kummer** *How does Gender Shape Science? The Entanglement of Scientific Competence and Fashion in Academic Physics*
	14:20 - 15:00	**Maria Rentetzi** *Women in Science: Why Should we Care?*
	15:00 - 16:30	**Coffee Break with Round-Table Discussion**
Session 7: Svetlana Tsogoeva	16:30 - 17:10	**Luzia Gyr** *Discovery of Antimicrobials Using High-Throughput Robotics*
	17:10 - 17:20	**Flash Talk: Julia Ryll** *Autofluorescent antimalarials by hybridization of artemisinin and coumarin: in vitro/in vivo studies and live-cell imaging*
	17:20 - 19:20	**Poster session and Finger Food**

Friday

Session 8: Claudia Vilhena	10:15 - 10:55	**Hannah Kurz** *Towards multifunctional zinc(II) coordination cages*
	10:55 - 11:05	**Flash Talk: Tamara Nagel** *Towards pecision controlled 2D functional group patterning of graphene via laser writing*
	11:05 - 11:45	**Grace Androga** *Re-imagining diagnostics to strengthen African health systems*
	11:45 - 12:00	**Award Ceremony and Closing Remarks**
	12:00	**Lunch and Farewell**

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Abstracts

Invited Speakers

Re-imagining diagnostics to strengthen African health systems

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My career has been shaped by a deep commitment to ensuring that scientific discovery translates into tangible benefits for people across Africa. From my early training as a medical scientist in Australia, I was drawn to the impact diagnostics can have on patient outcomes. This interest grew during my doctoral programme on *Clostridioides difficile* pathogenesis, where I built expertise in molecular microbiology and diagnostics, skills I have since applied to translational research on CNS and bloodstream infections.

Having lived in South Sudan, Kenya, and Uganda, and worked in Nigeria and now Malawi, I have gained first-hand insight into the realities of low-resource health systems, where the absence of accessible diagnostic tools can mean the difference between life and death. I was particularly struck by how anaerobic bacteria, despite their devastating role in wound and surgical infections, remain overlooked due to the lack of specialised facilities. These experiences fuel my determination to change the narrative. With support from the Thrasher and Wellcome Early Career Awards, I aim to advance diagnostic innovations, strengthen local capacity to improve patient care, and work towards a future where equitable diagnostics are the norm, not the exception.

Chemical biology for human health

Laura M. K. Dassama[1,2,3,*]

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[2]Department of Microbiology and Immunology, Stanford School of Medicine, Stanford, USA
[3]Sarafan ChEM-H Institute, Stanford, USA
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The ability to exert exquisite control of protein function remains a frontier in biomedicine. This is especially true for “undruggable” or otherwise challenging proteins that remain intractable to traditional occupancy-driven pharmacologies. This talk will describe the plethora of approaches employed by my research group, which include informatics, genetics, biochemistry, structural biology, and drug discovery campaigns, to uncover novel infectious disease targets. The talk will also highlight how protein engineering methods are leveraged to develop tools that exquisitely perturb the function of challenging disease relevant targets.

Discovery of Antimicrobials Using High-Throughput Robotics

Luzia Gyr[1,*]

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New and resistant human pathogens are spreading faster than suitable antimicrobial agents are developed. My independent junior research group, focuses on discovering novel compounds active against pathogenic fungi and bacteria using state-of-the-art high-throughput robotics. To that end, we have developed and established a modular lab automation system, which we termed JenXplor, as a novel technology platform at Leibniz-HKI. JenXplor enables innovative screening approaches to identify antibacterial and antifungal properties in compound libraries, with a primary focus on natural products. Beyond discovery, we investigate the mode of action of promising compounds and use the resulting data to train machine-learning models for the in-silico prediction of antimicrobial properties.
In addition to presenting our research, I will also share my journey from studying chemistry at ETH Zurich to becoming a junior research group leader at Leibniz-HKI. My path has shown me that pursuing what one truly enjoys not only drives scientific discovery but also opens doors to unexpected opportunities and growth.

Expanding the Druggable Space – My scientific journey through the rapidly evolving world of pharmaceutical research

Anastasia Hager[1,*]

[1]Bayer AG, Wuppertal, Germany
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Anastasia Hager will share her personal and professional journey. From her academic roots in chemistry at Würzburg and Berkeley, through her PhD in natural product synthesis at LMU Munich and postdoctoral work in chemical biology at Princeton, to her leadership roles at Bayer, Anastasia Hager illustrates how diverse experiences and interdisciplinary collaboration shaped her views on the rapidly evolving landscape of pharma R&D. As Head of Drug Discovery Sciences at Bayer Pharma, she leads cross-functional teams across different modalities, diverse assay and screening groups aiming to find the right molecule for the right target. Her talk will explore the challenges and breakthroughs in identifying novel mechanisms of action, promising lead candidates and how to optimize them.

Energy Management of Functional Molecular Materials

Helen Hölzel[1,2,*]

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The demand for sustainable energy solutions has intensified research into energy management, including harvesting, conversion, and storage. This work highlights functional molecular materials as energy storage systems upon photoexcitation. We discuss energy storage in chemical bonds and emphasize the photophysical properties essential for efficient energy use. Material preparation is briefly addressed, with focus on a semi-automated setup for rapid quantification of photophysical parameters, such as half-lifetimes and quantum yields. Proof-of-principle devices are presented, with emphasis on molecular solar thermal energy storage (MOST) systems - promising for solar energy harvesting and long-term storage.
MOST systems absorb sunlight and convert into energy-rich metastable isomers via photoisomerization, which can release energy on demand through a triggered back-reaction.[1,2] Flow chemistry, offering key advantages over batch processing, is applied for synthesis, optimization, and analysis.[3,4] Selected examples include norbornadiene/quadricyclane-based MOST systems.

References

[1] Z. Wang, et al, *Joule* **2021**, *5*, 3316.
[2] Z. Wang, et al, *Chem. Soc. Rev.* **2022**, *51*, 7313.
[3] J. Orrego-Hernández, et al, *Eur. J. Org. Chem.* **2021**, *2021*, 5337.
[4] N. Baggi, et al, *ChemSusChem* **2024**, *17*, e202301184.

Computational (photo)chemist at work: Is there only one way to do it right?

Joanna Jankowska[1,*]

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Being a computational chemist could be your dream research job in the 21st century. Your (virtual) lab is always within reach, and there is no such thing as expensive reagents or inefficient chemical synthesis. It seems that only your creativity and computing power could limit your scientific endeavors. But is this really true?

Let me share with you a story from one of our recent computational-photochemistry projects, concerning a reversible molecular motor. Light-driven rotary motors allow direct transformation of light energy into unidirectional rotary motion at the nanoscale. The key feature enabling the unidirectional rotation and controlling its direction is the motor's chirality – an inherently chemical factor, difficult to modify postsynthetically. In this project, we propose a new molecular rotary motor architecture, the **E-motor**, in which the motor's operating direction can be switched *in situ* with an external electric-field pulse, without the need for chemical modification of the system structure [1].

References

[1] K. Szychta, et al., *Sci. Adv.*, **2025**, *11,* eadt8008.

Design and Synthesis of Organic Electronic Materials

Malika Jeffries-EL[1,*], *David L Wheeler*[1]

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Over the past two decades, the number of consumer electronics has surged, increasing demand for semiconducting materials and energy. Traditional inorganic semiconductors rely on limited resources, prompting interest in organic alternatives. Organic semiconductors—polymers or small molecules with extended pi-conjugation—offer excellent electronic, optical, and thermal properties, making them ideal for transistors, solar cells, and LEDs. However, challenges remain before they can be widely commercialized. Our research group focuses on designing and synthesizing new organic semiconductors using low-cost, easily prepared starting materials. By tailoring their properties through chemical synthesis, we've developed novel aromatic building blocks, including wide-band gap materials for organic LEDs and narrow-band gap materials for photovoltaic cells. Our recent findings will be presented.

References

[1] D. L. Wheeler, et al., *Mater. Adv.,* **2022**, *3* (9), 3842-3852.
[2] D. L. Wheeler, et al., *J. Mater. Chem. C,* **2023**, *11* (1), 211-222.

Unravelling Metalloenzymes: Insights from Advanced EPR Spectroscopy

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Almost half of the enzymes require metals for their function. Therefore, it is tremendously important to understand how they utilize metals to perform complex oxidative/reductive chemistry. Electron paramagnetic resonance (EPR) spectroscopy is a powerful tool to study metalloproteins and has been central to our understanding of the fundamental processes in life. In my lab, we have been investigating the key metalloenzymes by employing advanced EPR methods combined with sophisticated bio-physical and -chemical tools.
In this talk, I will highlight our recent results on ribonucleotide reductases (RNR) and hydrogenases. RNRs play a fundamental role in cellular reproduction by catalysing the biosynthesis of DNA building blocks in every living cell. Hydrogenases catalyze the reversible conversion of molecular hydrogen into protons and electrons with remarkable efficiency. By employing advanced EPR techniques, we have gained valuable insights into the the intricate mechanisms underlying these enzymes' functions, thereby enhancing our understanding of their roles in critical biochemical processes.

Magnetoplasmonic Nanoparticles for X-ray triggered cancer therapy

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Radiosensitizers increase the susceptibility of tumors to radiation-induced injury. High atomic number nanomaterials such as gold nanoparticles enhance the effectiveness of conventional radiation therapy due to their high X-ray absorption coefficient. In cells, interactions of X-rays with drug-loaded superparamagnetic Fe_3O_4 nanoparticles causes the release of drugs into the cytosol. Simultaneously, X-ray radiation activates catalytic functionality of Fe_3O_4 surfaces. Surface standing Fe^{2+} and Fe^{3+} ions effectively catalyze Fenton and Haber-Weiss reaction. Due to alterations in reactive oxygen detoxifying enzyme levels, cancer cells often have elevated H_2O_2 levels. H_2O_2 is converted to highly toxic $OH^{\bullet}$ radical, so that the Fe^{2+} driven Fenton reaction is favored. However, under ambient conditions surface Fe^{2+} ions gradually oxidize to Fe^{3+} ions. Fe_3O_4 nanoparticles epitaxially grown on gold nanoparticles yielding Au-Fe_3O_4 nanoheterodimers retain Fenton catalytic activity [1-2]. In addition, X-rays release electrons from the gold component, leading to synergistic formation of reactive oxygen species.

References

[1] S. Klein et al, *ACS Appl. Mater. Interfaces.* **2018**, *10*, 17071-17080.
[2] S. Klein et al, *ACS Appl. Mater. Interfaces.* **2019**, *11*, 39613-39623.

Towards multifunctional zinc(II) coordination cages

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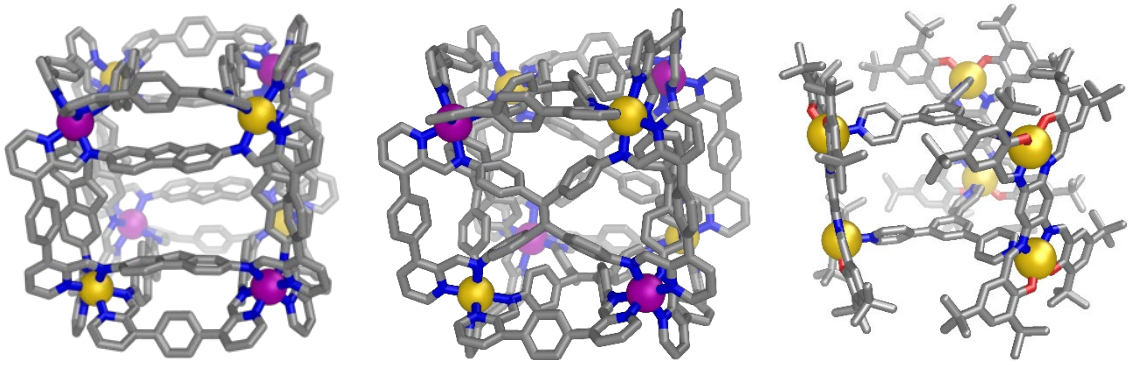
Photophysical and -chemical properties of molecules depend strongly on their local microenvironment. Bringing different photoactive units in a controlled manner in proximity can enable the targeted tuning of these properties. Coordination cages are promising systems for this purpose as they combine a simple synthesis by self-assembly with the chance to bring functional units into proximity in a highly controlled manner.
The first part of this talk reports on a new double-bridging strategy that enables the formation of highly stable zinc(II) cages. Besides the stability boost, this enables the incorporation of additional functional units into the cage scaffold. The second part focuses on the more traditional heteroleptic approach, which also allows bringing two functional units into proximity. As a new design principle, we utilize bissalophen units, therefore.



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Bridging Two Worlds – An Academic Journey between Research and Teaching

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My research interest centers on cardenolides and cardenolide derivatives, a group of bioactive plant natural products with a long history of medicinal use. Over the past years, we have investigated their biosynthesis in plants, focusing on enzymatic pathways and molecular mechanisms underlying the production of these compounds. This work has included the isolation and biochemical characterization of key enzymes, studies on metabolic regulation, and structure–activity analyses of cardenolides and derivatives. Beyond their classical role as cardioactive agents, cardenolides have demonstrated significant antiviral and anticancer activities, making them highly interesting for modern drug discovery. Therefore, we have studied their biological activities, particularly how subtle chemical modifications or glycosylation patterns influence their bioactivity. Insights into plant natural product biosynthesis and the knowledge of bioactivity and therapeutic potential of natural compounds can be integrated directly into lectures or lab courses for pharmacy and biology students. This creates an interdisciplinary learning environment where molecular processes, analytical methods intersect with the relevance of natural products research.

Chasing Dreams with a Little (Chiral) Twist

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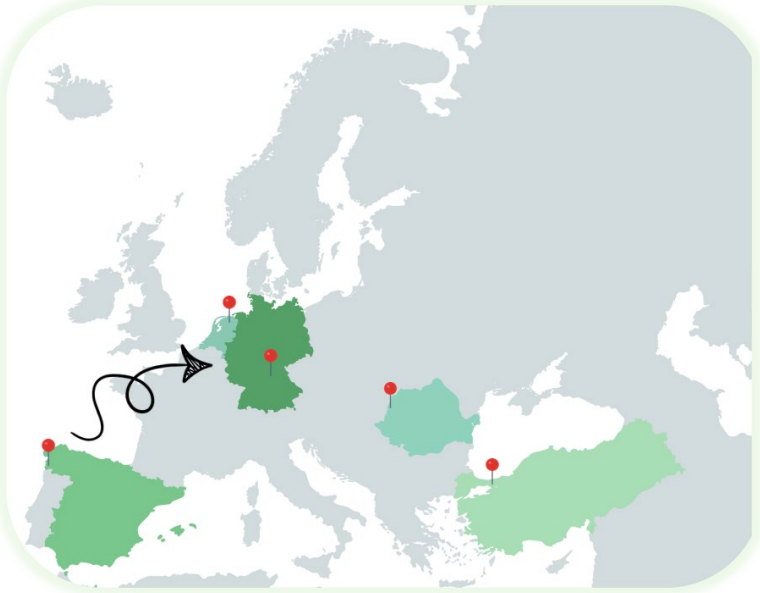
Chirality widely manifests itself in Nature at various hierarchical levels, expanding from tiny enantiomeric molecules to spiral galaxies at macroscopic level.[1] As molecules, light can be also chiral –referred to circularly polarized light– and its interaction with enantiomers give rise to chiroptical responses. Such fingerprint recognition feature is reminiscent of the *lock-key model* in terms of specificity and sensitivity.[2] Fascinated by this phenomenon and its uniqueness, my career journey has guided me along the different facets of chirality, including robust axially chiral small molecules[3,4] and macrocycles,[5] and ultimately the realm of molecular machines.[6,7]
My talk is thus divided into three sections: **(i)** *drivers* and *barriers* that I encountered while building up my career; **(ii)** some of my research highlights which marked and shaped my career journey; and **(iii)** as new and fresh chapter, transitioning from academia to research consultancy in order to assist other researchers, academicians, and industry experts in crafting highly competitive projects.



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Chemical Connections Between People: A Place for the Authentic You

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Life can sometimes take unexpected turns. It might be surprising to hear that I had zero interest in chemistry in childhood and most of adolescence, yet I ended up studying it, getting a PhD in it, becoming an editor at one of the prime chemistry journals in the world (*Angewandte Chemie*), and now working as a coordinating manager at the German Chemical Society (GDCh). What has driven these unconventional career decisions was the desire to find a good balance between working on the right thing and working with the right people. Human relationships are an essential part in the lives of scientists, and this talk aims to illustrate how societies like the GDCh contribute to building and fostering networks that bring joy and provide a place where everyone is comfortable to be their authentic self.

Figure 1. The German Chemical Society (GDCh) brings people together.

Coenzymes as connection between mineral-based and enzymatic catalysis en route to protometabolism

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The last universal common ancestor (LUCA) arose in an environment of rocks and water on the early Earth about 4 billion years ago. Top-down comparative bioinformatics reveal LUCA's carbon metabolism: the acetyl-CoA (or Wood-Ljungdahl) pathway, driven by CO2 and H2 gas1,2. Looking at abiotic, mineral-assisted organic syntheses occurring in hydrothermal vents today, we see how they resemble segments of the pathway3, possibly revealing LUCA's geochemical roots. In order to connect undirected, mineral-assisted catalysis with the complex enzymatic catalysis in LUCA (and extant biochemistry), we are zooming in on central metabolic organic cofactors, so helper molecules employed by enzymes. Examples also found in the acetyl-CoA pathway are nicotinamide adenosine dinucleotide (NAD), C1 donors and acceptors such as tetrahydrofolate (H4F) or, the namesake of the pathway, coenzyme A (CoA). Cofactors have been hypothesized to predate enzymes4, so in other words: cofactors could be the missing link between abiotic and biotic (enzymatic) catalysis.
We now show how cofactors employed in the acetyl-CoA pathway can function under conditions found in serpentinizing systems, where nickel- and iron-containing minerals transfer electrons to the protons of water, continuously producing hydrogen gas (H2) – LUCA's main electron and energy source. Not only can we show how activated hydrogen on minerals found in serpentinizing systems reduce the central redox cofactor nicotinamide adenosine dinucleotide (NAD)5, we can furthermore make assessments on how the structure of NAD enables specific reduction under geochemical conditions6. We were also able, only starting from H2, CO2 and nickel- and iron-containing minerals, to produce a cofactor-bound methyl-group, thus reproducing 50% of the acetyl-CoA pathway without enzymes. More than that, the according cofactor (H4F) is actively directing the CO2 fixation reaction with H2 towards methyl-group formation – thus catalyzing a metabolic reaction without the help of an enzyme. These results show how organic cofactors could play a central role in the transition between mineral and enzymatic catalysis.

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Women in Science: Why Should we Care?

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In early September 2025, Texas A&M University fired a professor who taught children's literature after accusations of promoting "gender ideology." The dean of the College of Arts and Sciences and the head of the department were also removed. The dismissals followed a student's recording of a classroom exchange, which began with her questioning the legitimacy of teaching about gender identity. She argued: *"According to our president, there are only two genders, and he said he would be freezing agencies' funding programs that promote gender ideology. This also goes against not only my own beliefs but also those of many people's religious convictions."* As academic freedom in U.S. universities faces increasing challenges and gender studies get under serious scrutiny, I would like to turn to the life and work of one of the most renowned women in physics, Lise Meitner, and reflect on why it is essential to care about women in physics and gender in general.

Flash Talks

With my feet in the air and my head on the ground

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"Analog missions" are an experimental approach to study effects of space environments on hardware, crew and individual astronauts. They take place in locations that have natural or engineered physical similarities to extreme conditions in space at costs ranging from several hundreds of thousands to some tens of millions of euros per mission. Travelling through academia, on the shoulders of giants who feed the world or travel the galaxy, I noticed a striking parallel: "*being a post-doc is pretty much like participating in the most realistic and large-scale analog mission in the history of space research.*" While this statement and the topic of the talk is a) not really at the core of my expertise, b) probably not among the most hard-core scientific presentations of this symposium, and c) is likely to appear far-fetched initially, I would like to present and discuss some of the curious parallels, sometimes hilarious, and partially dramatic analogies that led me to this comparison.

Structural and spectroscopic characterisation of AlkB domains involved in electron transfer during alkane oxidation

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Biological alkane oxidation plays a critical role in the global carbon cycle by enabling microorganisms to metabolise up to 800 million tons of hydrocarbons annually. However, alkanes are chemically inert and challenging to functionalize selectively. Nature has evolved alkane-oxidising systems (AlkBGT) that can selectively hydroxylate terminal C–H bonds of liquid alkanes. Here, we present structural and spectroscopic data on three distinct electron transfer systems associated with AlkB enzymes, each with diverse protein architectures. Spectroscopy of the electron transfer domains shows that rubredoxin-type centres are typically employed; however, we unexpectedly discovered that a ferredoxin-type [2Fe-2S] cluster can also mediate electron transfer. Additionally, we solved the crystal structure of an NADH-dependent reductase domain, providing insight into the electron transfer step. The presence of different forms of AlkB in these organisms suggests evolutionary ways to improve electron-transfer strategies to AlkB. The knowledge of structural and functional properties of various Fe-S binding sites, as well as overall domain architecture, enables us to engineer more efficient biocatalysts for applications related to environmental bioremediation.

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Tuning the Transparency and Exciton Transition of D-π-A-π-D Type Small Molecules

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Organic small molecules possess significant potential for semitransparent optoelectronic applications due to their tunable optical properties and inherent transparency. However, tailoring these materials is challenging as their optoelectronic properties are sensitive to subtle structural changes, compounded by the existence of over a million potential structural designs. To address these complexities, we present a material discovery workflow that combines literature-based molecule preselection with TDDFT calculations, creating customized small molecule structures with adjustable transparency windows. We identified fifty-four small molecules with a D-π-A-π-D architecture, incorporating nine central (A) and six end (D) units connected by a thiophene π-bridge. Through TDDFT calculations, we determined the theoretical absorption spectra and energy levels of the identified molecules. Ultimately, we synthesized twenty-four molecules that exhibit promising transparency properties by selectively absorbing photons in the ultraviolet (UV) and near-infrared (NIR) regions, with a significant optical transmission band relevant to the visible spectrum which we will refer to as “optical window”. Characterization of the resultant small molecules revealed that six of them, in particular, exhibited selective absorption with the broadest “optical window”. We believe that our study will provide valuable insights to establish effective material discovery workflow for highly transparent conjugated organic small molecules.

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How does Gender Shape Science? The Entanglement of Scientific Competence and Fashion in Academic Physics

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In our talk, we discuss the process and results of our research project on "The Entanglement of Scientific Competence and Fashion in the Field of Physics in Academia." Using structured interviews conducted with senior researchers from various fields of physics, we sought to answer the following question: What role does attire play for professors in the field of physics in an academic environment, and are there gender-specific differences? The objective was to examine established gender norms and performative behaviors in a scientific field that considers itself "gender neutral." In particular, the study aimed at exploring how individuals navigate and interpret potential conflicts between personal expression and the expectations of a scientific persona. In our results, we were able to clearly identify gender-normative constraints and behaviors regarding professional self-representation and the scope of "doing gender." The findings highlight that attire exists in a superposition, simultaneously influencing and reflecting perceptions of competence, leadership, and belonging, uncovering the complex social and cultural forces through which gender continues to shape science [1].

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Autofluorescent antimalarials by hybridization of artemisinin and coumarin: in vitro/in vivo studies and live-cell imaging†

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Malaria is one of the most widespread and deadliest diseases, with an ever-consistent need for new and improved pharmaceuticals. Natural products have been an essential source of hit and lead compounds for drug discovery. Antimalarial drug artemisinin (ART), a highly effective natural product, is an enantiopure sesquiterpene lactone and occurs in Artemisia annua L. The development of improved antimalarial drugs, which are highly potent and fluorescent, is particularly favorable and highly desirable for live-cell imaging, avoiding the requirement of the drug's linkage to an external fluorescent label. Herein, we present the first antimalarial autofluorescent artemisinin-coumarin hybrids with high fluorescence quantum yields of up to 0.94 and exhibiting excellent activity in vitro against CQ-resistant and multidrug-resistant P. falciparum strains. Furthermore, a clear correlation between in vitro potency and in vivo efficacy of antimalarial autofluorescent hybrids was demonstrated. Moreover, these hybrids were not only able to overcome drug resistance, they were also of high value in investigating their mode of action via time-dependent imaging resolution in living P. falciparum-infected red blood cells.

Towards precision controlled 2D functional group patterning of graphene *via* laser writing

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The chemical structuring of 2D materials such as graphene enables the specific tailoring of its outstanding properties and due to this, is of uttermost interest for the development of high-performance 2D materials. By applying covalent functionalization with local control, adjacent domains with altering chemical and physical properties can be generated, allowing for a complex pattern design. The so-called laser 'writing' is one of the most promising approaches to achieve this goal. Here, a chemical reaction is locally triggered by a freely movable stimulus such as laser irradiation, allowing for a site-selective functionalization of graphene. We herein present a significant advance in the understanding of the reaction mechanism and the influence of the laser 'writing' parameters in the laser-triggered activation of dibenzoyl peroxide (DBPO) and the subsequent high-precision covalent patterning of functional groups on monolayer graphene.[1-2]

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Poster Abstracts

Polyelectrolyte-Directed Platinum Nanostructures for Catalytic Applications

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This project investigates the formation, structure and catalytic behavior of platinum nanostructures within two polyelectrolyte systems: a custom-designed phosphonated fluorinated polystyrene and commercial poly(styrene sulfonate) (PSS). The goal is to design novel systems for photocatalysis. We use “electrostatic nanotemplating to create particles in aqueous solution: Dicationic tetraammineplatinum(II) ions accumulate inside the oppositely charged polyelectrolyte and controlled reduction using sodium borohydride ($NaBH_4$) was employed to synthesize platinum nanoparticles within the polymer matrix. For exploiting their function, it is important to understand how platinum ions (Pt^{2+}) interact with negatively charged polymer chains in aqueous solutions. By varying the polymer concentration and the Pt^{2+}/polymer charge ratio, we monitored changes in hydrodynamic radius using dynamic light scattering (DLS) and evaluated the extent of metal ion binding and subsequent reduction. Results reveal that both polyelectrolytes exhibit distinct binding and aggregation behaviors due to their differing charge densities and backbone structures. Post-reduction analysis confirmed nanoparticle formation, with optimal stability observed at intermediate charge ratios. These particles are currently tested as novel catalyst systems. This study provides insights into the templating role of polyelectrolytes in nanomaterial synthesis systems for various possible future catalytic or functions and applications.

Acknowledgment

We gratefully acknowledge Dr. Maximilian Wagner (Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien) for providing the custom-designed polymers used in this work.

Cell shape and division septa positioning in filamentous *Streptomyces* require a functional cell wall glycopolymer ligase CglA

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Streptomyces are soil-dwelling Actinomycetota, renowned antibiotic producers displaying complex life cycle transitioning from filamentous vegetative mycelia to spores[1]. This process is tightly regulated by cell envelope biogenesis to sustain morphology, viability, and development. Cell wall of Gram-positive bacteria consists of a thick peptidoglycan layer with covalently attached glycopolymers, essential for integrity, shape, and vitality. *Streptomyces* proliferate via apical extension and hyphal branching, that require proper localization of cell wall machinery; however, the composition and regulation of their envelope remain poorly understood. We identified the LCP-LytR_C domain protein CglA as a key glycopolymer ligase in *S. venezuelae* that localizes to cell wall biosynthesis zones, and its mutation diminishes glycopolymer content, disrupts FtsZ-ring positioning, and produces enlarged hyphae with mispositioned septa and defective spores. Notably, we reveal a physiological link between c-di-AMP signaling and cell wall glycopolymer decoration, as *cglA* inactivation rescues the salt-sensitive phenotype of the *disA* mutant. These findings establish CglA as a novel determinant of cell wall biogenesis critical for *Streptomyces* vitality.

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Advancing Light-Induced Bidirectional Photoswitching of Norbornadiene

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The norbornadiene/quadricyclane (NBD-QC) photoswitch is a promising candidate for molecular solar energy storage. Isomerization to the energy-storing, metastable QC occurs upon UV light irradiation, while the back-switch can be triggered in various ways. To date, performing complete, on-demand energy release across multiple switching cycles remains a significant challenge in molecular solar thermal (MOST) research.[1] We demonstrate the implementation of perylene diimide (PDI) as photoactive redox catalyst to trigger energy release upon 475 nm irradiation. Investigation of the switching properties of several *imide*- and *ortho*- connected NBD-PDI hybrids revealed a low effect of varying the connection positions on the isomerization efficiency. Concentration-dependent studies identified an alternative intermolecular mechanism for back-switching in addition to the previously known intramolecular pathway. Advancing exclusively photoinduced NBD/QC isomerization in novel NBD-PDI hybrids establishes the foundation for targeted manipulation of photoswitch systems forapplications such as energy storage. Their autonomous operation principle makes hybrid systems particularly interesting for molecular solar energy storage research.

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Spatially Resolved Covalent Functionalization on Graphene and (6,5)-SWCNT's *via* Laser Writing

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Modifying graphene and single-walled carbon nanotubes (SWCNT's) *via* covalent functionalization by introducing various functional moieties and therefore tuning the chemical properties has established itself as a key field in research.[1-2]Modern 2D patterning techniques, which combine highly efficient, covalent functionalization with precise spatial resolution, allows for a dimensional and quantitative control over the addend binding.[3]Herein, we present an optimized protocol for the laser-activated spatially resolved functionalization of graphene using various diazonium salts exhibiting different functional groups. Furthermore, we successfully transferred the well-established 'laser writing' protocol to covalently functionalize a thin film of (6,5)-SWCNT's with various reactive moieties.

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

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The Gram-positive human pathogen *Streptococcus pneumoniae* adapts its metabolism to the environment during host invasion. Extracellular vesicles are produced by *S. pneumoniae* (Sp-EVs) during this process, but the exact interplay between metabolic adaptation and vesicle formation remains elusive. We characterized EVs isolated from *S. pneumoniae* D39, grown under different environmental conditions (human serum, temperature, pH and glucose availability), using nanoparticle tracking analysis. To study Sp-EVs protein cargo, a proteomic and a functional interaction analysis were conducted. Biofilm formation was assessed to investigate Sp-EVs role in intra- and inter-species communication.We demonstrate that exposure to normal human serum and low glucose availability significantly increased Sp-EVs production. Carbon metabolism pathways were enriched in Sp-EVs proteome. Functionally, Sp-EVs promoted biofilm formation in both *S. pneumoniae* and *Streptococcus pyogenes*. By exploring how environmental conditions shape pneumococcal EVs production and function, our study contributes to the understanding of *S. pneumoniae* infection, with potential future applications in therapies.

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OVERCOMING AMPHIPHILIC AND NON-EQUILIBRIUM SELF-ASSEMBLY OF ORGANIC SEMICONDUCTOR THIN FILMS AT THE SOLVENT-WATER INTERFACE

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Recent advances in solution-based processing have enabled significant progress in organic thin-film fabrication for electronic devices. Previously, we reported successful polymer monolayer fabrication via the Langmuir-Blodgett (LB) technique at the air-water interface.[1] Here, we demonstrate a liquid-liquid interface self-assembly approach for fabricating high-quality crystalline thin-films of the organic semiconductor C13-BTBT. This method relies on intermolecular forces at the boundary of two immiscible liquids. By controlling the temperature and maintaining a saturated solvent/N_2 atmosphere, we allow sufficient time for π-π interactions to guide uniform crystalline film formation. The formed layers exhibit lateral diffusion on the water surface, promoting azimuthal reorientation into single-crystalline domains. Film formation is monitored in-situ using light microscopy with real-time capturing. Through optimization of the experimental conditions, we achieved reproducible formation of large-area C13-BTBT thin-films (2x2 cm²), surpassing the structural quality and size of films obtained by conventional techniques.[2]

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Mapping the Gas Channel in the [FeFe] Hydrogenase from N. vulgaris

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Hydrogen gas is an environmentally sound energy carrier with high energy density. Hydrogenases are metalloenzymes found in nature that very efficiently catalyze the reversible reduction of protons to molecular H_2. The oxygen-sensitive active site is buried deep within the enzyme, requiring gas molecules including oxygen to access it through an internal channel. Here, we map the gas channel of the [FeFe] hydrogenase from *Nitratidesulfovibrio vulgaris* (*Nv*HydAB) using a high-pressure freezing technique to derivatize protein crystals with krypton. In the obtained XRD structures, up to four krypton atoms were located within the proposed cavity in the protein, identifying it as the putative gas channel used by *Nv*HydAB. Subsequent mutations of selected residues in the channel demonstrated that site-directed, rational modification is possible without affecting the overall conformation of the hydrogenase. Therefore, our findings provide insight into gas transport in *Nv*HydAB and offer exciting new opportunities for modulating the enzyme's properties, particularly in efforts to protect it from degradation by O_2.

Breaking the Code: DNAzyme-Mediated Cleavage of HIV-1 Gag RNA

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DNA enzymes (DNAzymes) are promising gene-silencing agents for treating genetic disorders, infectious diseases and cancer. They offer advantages over other gene-silencing methods, such as siRNA, due to their high stability, multiple turnover rates and ready availability. We designed four 10-23 DNAzyme variants targeting HIV-1 Gag RNA. Cleavage assays on short RNA sequences confirmed Mg^{2+}-dependent activity of the DNAzymes, with varying efficiencies among variants. Further, our 10-23 DNAzymes cleaved full-length in vitro RNA transcripts, demonstrating the efficiency and great gene-silencing potential of our design.

Nanodevices for pH sensing and control in microliter-scale bioreactors

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Bioprocesses are moving into focus of industrial production processes to enable sustainable syntheses. However, their development remains highly time-, resource-, and cost-intensive [1]. Although experiments have been highly parallelized and miniaturized, they are often limited in the controllability of key parameters such as pH, which is crucial for bioreactions. To address this, we aim to establish a polymersome-based nanodevice for pH sensing and control at the microliter scale. The polymersome is functionalized with inserted proteins for sensing the environmental pH and transmitting the signal to an external detector. By inserting a pH-sensitive fluorescent protein, the pH shift becomes externally detectable and serves as a basis for pH adjustment. Upon illumination, a light-driven proton pump then transports protons across the membrane [2].

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Investigation of the interlayer coupling of twisted bilayer MoS2 and MoSe2 via Raman spectroscopy

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Stacking two monolayers of TMDCs on top of each other introduces several novel phenomena as, e.g.,the formation of moiré phonons and might change the band structure. In addition, the fabrication process and the twist angle both influence the coupling between the two layers. Here, this interlayer coupling is investigated via Raman spectroscopy. By exciting the C exciton resonance, interlayer Raman modes are activated that are not visible in a single layer but become active in bilayers. This is because the C exciton - in contrast to A and B excitons - expands over both layers and, therefore, couples the layers electronically. Taking well-coupled twisted bilayer samples as a starting point we investigate the influence of the twist angle on the C exciton resonance by taking Raman spectra of several samples with different twist angles at different laser excitation energies. All measurements have been done using twisted bilayer MoS2 and MoSe2.

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

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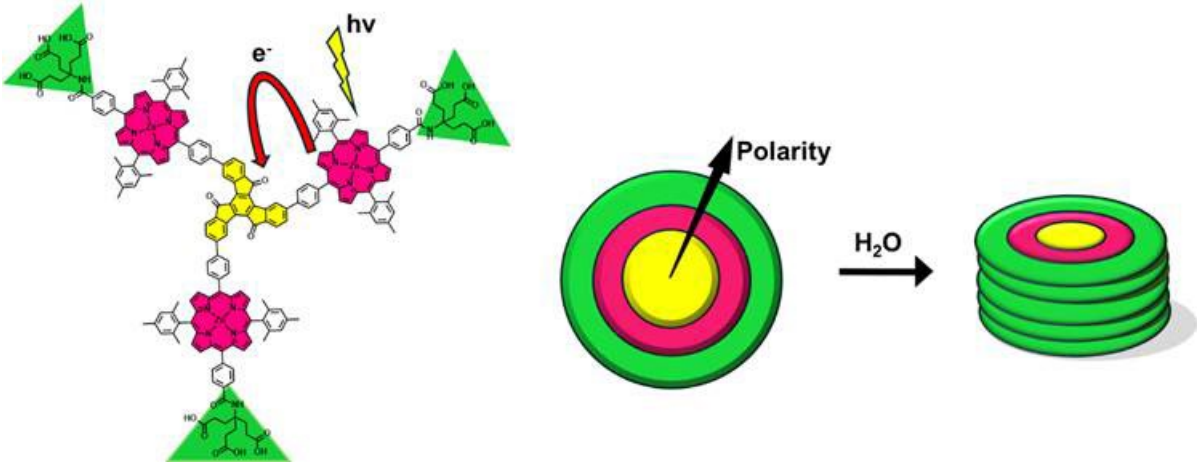
Porphyrins have already been used as efficient donor moieties in architectures with carbon-rich acceptor moieties such as fullerenes to generate photoinduced charge separation.[1] Here, we present the synthesis of novel discotic amphiphilic porphyrin-PAH conjugates, where a PAH is used as the central fragment, which is functionalized on its periphery with zinc-porphyrins. These in turn, possess Newkome-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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Triazine-naphthalimide receptors for the recognition of Fluoride and GTP

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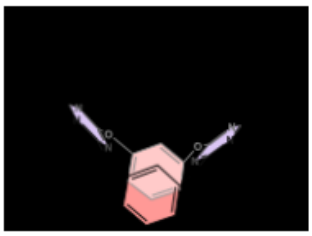
Triazine-based hosts have attracted interest in recent years because of their electron-deficient systems which can efficiently coordinate anions [1]. We designed and investigated properties of the new fluorescent triazine-based macrocycles. Due to their electron-deficient nature, they can bind both small and large anions. For example, we found that receptor 1, in which a triazine macrocycle is directly connected to two naphthalimide dyes, can change its color and fluorescent properties in the presence of fluoride anions in organic solution. This change is attributed to the formation of a charge-transfer complex. To examine the ability of triazine-based systems to interact with nucleotide [2,3], we synthesized receptor 2 with amine groups. These groups carry positive charges in water and contribute to good solubility. This receptor demonstrated the ability to selectively bind guanosine triphosphate and G-quadruplex. The macrocycles binding interactions were characterized using spectroscopic techniques, revealing a district fluorescence response upon Fluoride and GTP recognition (Figure 1).



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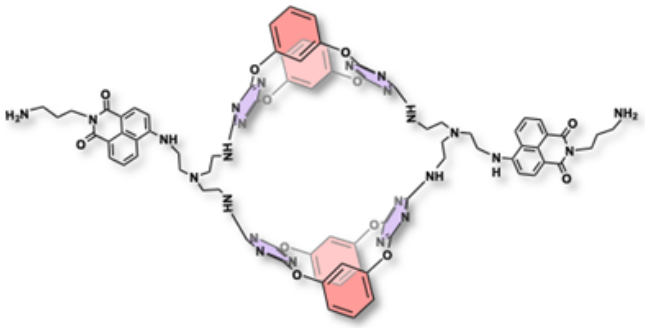

(2)

Figure 1: Structure of triazine-naphthalimide receptors for detection of Fluoride (1) and GTP (2).

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Synthesis of π-Extended Triptycene Porphyrin Hybrids for Host-Guest Assemblies

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The extension of the π-system of porphyrins has received high attention in the field of organic electronics.[1] Interestingly, Scholl Oxidation has shown to be a useful method for expanding the π-system of porphyrins, observing a new electronic structure of the parent porphyrin.[2] Furthermore, the π-extension of porphyrins could possibly improve their binding abilities in supramolecular structures. In this project, triptycene, commonly used in supramolecular chemistry,[3] was connected to the porphyrin in the meso-position. In the last step, Scholl Oxidation of triptycene porphyrin derivatives NiPorTrp and NiPorTrp2 led to a bond formation the beta-position yielding fNiPorTrp and fNiPorTrp2 (Figure 1).
UV-Vis spectroscopy of the fused porphyrins revealed a drastic change in absorption similar to those in literature.[2] In addition, the pincer-like shape of fNiPorTrp2 makes it a promising candidate for binding fullerenes in supramolecular clusters.

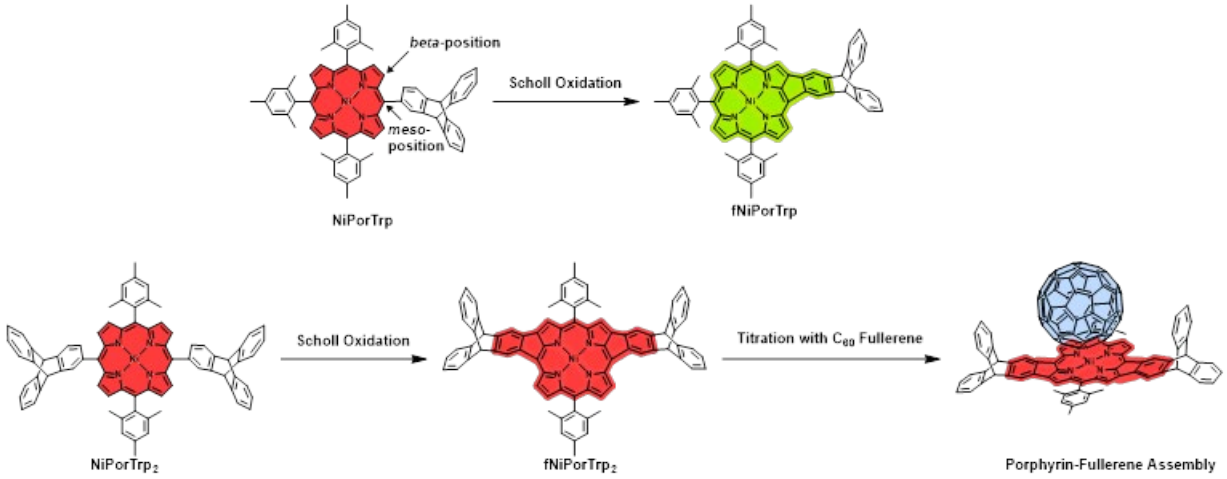

Figure 1. Synthesis Approach of fused Triptycene Porphyrin conjugates.

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Additive manufacturing of graphitic carbon nitride composite electrodes for photocatalytic degradation applications

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Fused deposition modeling (FDM) based 3D printing is becoming more relevant for fabricating photocatalytic electrodes. Fabrication of multi-material filament enables tailoring the specific properties of filament and hence the final electrodes for desired applications.[1] By using a photocatalytic semiconductor such as graphitic carbon nitride (g-C_3N_4), functionalized with carbonized polydopamine (cPDA) and incorporating them into a polylactic acid (PLA) matrix, we produced composite filaments for printing electrodes. We used these electrodes under simulated sunlight for the degradation of a commonly used dye found in wastewater. These electrodes offer an easy and convenient handling, as it is otherwise difficult to recover material in its powder form.[2] We show the possibility of upscaling by demonstrating that using electrodes with a larger surface area leads to a linear increase of degradation performance.

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Synthesis And Characterization of Zn-Based Metal-Organic Frameworks for Supercapacitor Applications

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Supercapacitors have attracted attention for their efficient short-term power delivery, but issues like low storage capacity and poor stability limit their performance. Metal-organic frameworks (MOFs), with large surface areas and many redox sites, offer promising solutions. In this study, Zn/M^{2+}-MOF (M = Cu, Co) electrodes were synthesized using microwave-assisted methods and tested for supercapacitor applications. Zinc-based MOFs with copper and cobalt were prepared at different ratios (4:1, 2:1, 1:1, 1:2, 1:4) and characterized by XRD, SEM, FT-IR, UV-Vis, and EDX. Structural analysis showed distinct compositions and crystalline structures. Electrochemical performance was examined through galvanostatic charge-discharge (GCD), cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS). The 2:1 Zn/Cu-MOF and 1:1 Zn/Co-MOF samples exhibited the highest capacitance of 164 F/g and 464 F/g at 5 mV/s, along with energy densities of 20.5 Wh/kg and 58 Wh/kg, and power densities of 978 W/kg and 8540 W/kg, respectively. Both maintained excellent cycling stability, retaining 99% and 96% of their capacitance over 2000 cycles, demonstrating their potential as efficient electrode materials.

Keywords: Electrode materials, Metal-organic frameworks (MOFs), Supercapacitors.

Comparison of two AMBER force fields regarding structural changes in pH-responsive helical peptides

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pH-induced structural changes are a common mechanism in physiological[1] and pathological[2] processes, and in the design of biomaterials[3]. These changes often involve the formation or unfolding of α-helices facilitated by altered protonation states of titratable side chains. We employed molecular dynamics simulations to investigate how ionically stabilised peptides respond to changes in the protonation state of their titratable residues. Our study focuses on comparing two AMBER force fields (ff14SB and ff19SB), providing a comprehensive benchmark analysis of their similarities and differences. While the overall trend in structural behaviour is similar between the two force fields, differences become apparent when examining specific properties, such as the number of hydrogen bonds formed. Our work provides a basis for research involving pH-responsive α-helical peptides and highlights the importance of choosing force fields that are appropriate for one's project.

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Development of an Organoautocatalyzed Double σ-Bond C(sp 2)-N Transamination Metathesis Reaction

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The transamination reaction, which involves the conversion of one amine to another, traditionally relies on biological enzyme catalysts. Although chemists have recently developed a few transition metal-catalyzed methods, mimicking these enzymes to interconvert amine groups in acyclic substrates via transamination metathesis of a single C(sp^2)–N bond, transamination of cyclic tertiary amines has remained a challenge in synthetic chemistry. Here, we present the development of organoautocatalyzed transamination metathesis of two C(sp^2)–N bonds in a cyclic substrate that allows for the challenging transformation to take place with up to 95% yield under exceptionally mild reaction conditions at room temperature without external catalysts and/or additives. The reaction mechanism has been studied in detail through time-resolved ^{1}H-NMR, 2D NMR, and computational methods. Remarkably, in situ-formed pyrrolidinium salt acts as a hydrogen bond donor (HBD) organoautocatalyst in this multi-step domino process. The new organoautocatalyzed methodology gives environmentally friendly, atom-economical, straightforward, and rapid access to N-substituted 3,5-dinitro-1,4-dihydropyridines (DNDHPs), thus offering facile entry to privileged bioactive compounds.

Green Synthesis of New Highly Functionalized Quinolines *via* Novel Fe(III)-Catalyzed Domino *aza*-Michael/Aldol/Aromatization Reaction

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Quinoline heterocycles, widely found in pharmaceuticals and drugs, exhibit diverse biological activities ranging from antifungal and antibacterial to antiviral effects against pathogens such as coronaviruses, HIV, and flaviviruses.[1] Recently, we reported the development of a straightforward, waste-reducing, environmentally friendly Fe(III)-catalyzed domino aza-Michael/aldol/aromatization reaction in the presence of water to access high-value functionalized quinolines using 2-aminobenzophenones and ethyl buta-2,3-dienoate as starting compounds.[2] The tangible advantages, i.e., utilization of commercially available and/or easily accessible substrates, simplicity, and mild reaction conditions, make this green three-step domino process highly appealing for the direct construction of a wide variety of highly functionalized quinolines in up to 78% yield. These results will be discussed in the presentation.

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ST171, a novel 5-HT$_{1A}$ receptor agonist for the treatment of pain

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The 5-HT$_{1A}$ receptor is a promising target for pain management [1]. Here we present compound ST171, which demonstrates strong pain-relieving effects *in vivo*. Using luminescence-based cAMP assays, ST171 was shown to exclusively activate G$_{i/o}$pathway in the HEK293T cells. A knock-out cell line strategy and kinetic studies further confirmed this selective activation. To explore G$_{i/o}$ subtype selectivity, we tested ST171 along with α_{2A} adrenergic receptor analgesic agonists PS75 and '9087 [2] in HEK293AΔGi cells co-transfected with subtypes of the G$_{i/o}$ family. All compounds show E$_{max}$ preference for Gα_z and Gα_{oA} subunits. Our findings show that ST171 is a functionally selective G$_{i/o}$ agonist and suggest that coupling to Gα_{oA} and Gα_z may be important for more effective pain therapies.

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Early-Stage Nucleation in Electrochemical Atomic Layer Deposition: Se Deposition on Au(111)

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Electrochemical atomic layer deposition (EC-ALD) enables the fabrication of semiconductor thin films, such as In_2Se_3 [1], with atomic-level thickness control while maintaining conformality and the advantages of a solution-based process. ALD requires self-limiting reactions, which can be realized 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. However, the defect density of the semiconductor thin film is largely determined by the initial nucleation behavior.
In this work, we investigated the initial nucleation of an EC-ALD half-cycle—the deposition of Se on Au(111)—using in-situ electrochemical atomic force microscopy (EC-AFM) and cyclic voltammetry (CV). We identified three potential growth regimes: UPD (+0.34 – +0.46 V_{RHE}), a mixed UPD/bulk deposition region (-0.02 – +0.34 V_{RHE}), and bulk deposition (below -0.02 V_{RHE}). Our study provides a comprehensive picture of how the film morphology evolves over time across different growth regimes.

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Exploration of the early stages of silica formation with potentiometric titration

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Silica crystallization processes are important for geochemical and protobiological processes; however, the molecular mechanisms underlying phase separation and the formation of first solid states in homogeneous aqueous solutions is unknown. It is hypothesized that during the first 500 million years of Earth's history, known as the Hadean period, the waters were rich in silica. Understanding silica formation is essential for elucidating the formation of biominerals that life developed on the early Earth. Laboratory experiments are designed to simulate Hadean conditions through potentiometric titration experiments, which control the silica precipitation involving pre-nucleation clusters by using waterglass as precursor. Titration experiments conduct under constant conditions including pH value, concentration and dosing rate, reveal the pH dependency of silica precipitation.

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In-Situ Electrolyte for Electrosynthesis: Scalable Anodically-Enabled One-Pot Sequence from Aldehyde to Isoxazol(in)es

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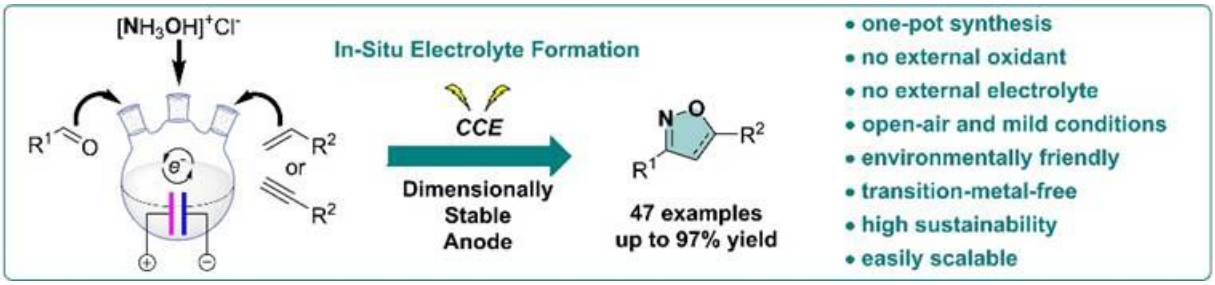

Electrochemical transformations are considered a green alternative to classical redox chemistry as it eliminates the necessity for toxic and waste producing redox reagents. Typical electrochemical reactions require the addition of a supporting electrolyte – an ionic compound to facilitate reaction medium conductivity. However, this is often accompanied by an increase in the amount of produced waste. Here, we report an "in-situ electrolyte" concept for facile, transition-metal-free, additive-free one-pot electrochemical preparation of isoxazol(in)es, important scaffolds for biologically active natural and synthetic molecules, from the respective aldehydes. The protocol utilizes no halogenated solvents and no external oxidants, while salt side-products provide the ionic conductivity necessary for the electrosynthesis. The electrolysis is performed in an undivided cell, using the state-of-the-art electrodes for the chlor-alkali industry dimensionally stable and scalable mixed metal oxide anode and platinized titanium cathode of high durability. The cascade transformation comprises the condensation of aldehyde to oxime followed by its anodic oxidation and subsequent intra- and/or intermolecular [3+2] cycloadditions with an appropriate dipolarophile. Chemical yields up to 97 %, and good Faradaic efficiency, scalability, and stability are observed for most substrates in a broad scope.

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Key Aspects Toward Realizing a Photocathode for Photoelectrochemical CO_2 Reduction

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Artificial photosynthesis, the combination of water oxidation and carbon dioxide reduction in a photoelectrochemical cell, is a promising route for more sustainable fuel production and solar energy storage. Herein, the key aspects for realizing a photocathode for solar-driven CO_2 reduction are presented.

Essential for such reduction reactions is the efficient generation of charge carriers, which is obtained by using quantum dots (QDs) as a light-absorbing material. QDs are particularly promising since their optoelectronic properties can be tuned during the synthesis or in the following processing steps, making them a flexible platform to optimize device performance on a laboratory scale. We study $CuInS_2$ QDs as a ternary chalcogenide material of comparably low toxicity, based on relatively earth-abundant elements, to enable renewable energy concepts.

Using nanostructuring to systematically enlarge the active surface area promotes efficient material usage without requiring macroscopic sample scale-up. Combining $CuInS_2$ QDs as photoactive component with thin layers of functional transport materials and a suitable catalyst offers an ideal framework for understanding and steering the mechanisms of solar-driven electrocatalysis.

Solution-processed NiO materials for urea oxidation – the role of morphology and electronic structure

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Non-precious NiO exhibits catalytic activity toward the urea oxidation reaction, making it an attractive alternative to the kinetically slow oxygen evolution reaction in coupled redox systems. Precise and versatile size and shape control can be achieved by solution-based nanoparticle syntheses, minimizing material consumption and maximizing the nanoscale active surface area. These catalyst nanomaterials have demonstrated promising electrochemical performance; however, downsizing induces fundamental transformations in their electronic (defect) structure compared to their bulk counterparts.

We successfully synthesized spherical, crystalline NiO nanoparticles, whose electrocatalytic affinity towards water and urea oxidation was studied using current-voltage and impedance techniques. These results were correlated with their optoelectronic defect structure, probed by transient absorption spectroscopy, revealing that intra-bandgap states directly govern charge transfer resistances.

Ongoing work focuses on tailoring surface chemistry through ligand engineering, specifically by exchanging and/or removing long-chained ligands from the synthesis with short-chained analogues to establish a mechanism framework for nanomaterial catalysis.

This research aims to directly couple optoelectronic properties with surface chemistry and electrocatalytic performance, advancing the design principles for tunable nanocatalysis.

PHYDINE: Advancing Diversity in Academia for Diversity of Academia

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Diversity in natural sciences is a matter of scientific progress: a wider range of perspectives fosters creativity and innovation – essential traits in academic research. However, barriers such as inaccessible infrastructures, cultural and gender biases still limit participation in academia. Addressing these challenges requires intersectional and interdisciplinary approaches, allyship across all career stages, and institutional commitment to inclusive practices. At FAU Erlangen-Nuremberg, the Physics Diversity Network (PHYDINE) seeks to put these principles into practice. By organizing round tables, discussion rounds, and the biannual DIPHER conference, the PHYDINE working group is active in raising awareness within the FAU physics department and online via social media, and creates spaces for discussing topics related to gender, cultural perspectives, neurodiversity, and accessibility in academia. By driving initiatives such as the movement for free hygiene products and special needs toilets, PHYDINE contributes to a more inclusive environment at FAU. Taken together, PHYDINE demonstrates that diversity in physics is vital for the diversity of physics and thereby sets an example for advancing diversity in academia[1].

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Synthesis of Adamantane-Scaffold-Containing Derivatives via the Ugi Four-Component Reaction

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Adamantane-containing derivatives are a privileged class of scaffolds in medicinal chemistry due to their diverse biological activities and unique physicochemical properties. The rigid, lipophilic cage-like structure of adamantane enhances drug-like behavior by improving membrane permeability, metabolic stability, and target affinity. In this study, novel adamantane-functionalized peptidomimetics were synthesized via the Ugi four-component reaction (U-4CR), an efficient multicomponent strategy that rapidly generates molecular diversity in a single step. The approach employed adamantane-based building blocks, including adamantane-1-carboxylic acid, 1-aminoadamantane, adamantanone, and aryl/alkyl isocyanides, combined with aldehydes and carboxylic acids, yielding a library of peptidomimetics incorporating adamantane moieties. The synthesized compounds were structurally characterized, and selected derivatives were assessed for antimicrobial activity against ten clinically relevant bacterial strains using the disk diffusion method. These findings demonstrate the synergy between adamantane pharmacophores and multicomponent chemistry, establishing the Ugi reaction as a versatile platform for creating multifunctional bioactive molecules with promising therapeutic potential.

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Formation of highly porous silver from crystalline and amorphous silver citrate

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Silver is a noble metal with unique physical and chemical properties. Its extensive use across various fields attracts attention and broadens its possibilities [1]. These capabilities largely depend on the surface and different morphologies of silver nano- and microparticles. Porous silver is a type of material that contains many interconnected pores or voids within its structure. These pores are usually on the nanoscale, ranging from a few nanometers to a few micrometers, which makes the sample suitable for producing porous silver using the potentiometric titration method. During this process, we aim to understand the mechanism of nucleation of silver citrate. However, many questions about the early stages of silver citrate formation remain unanswered, and it is unclear whether nucleation follows classical nucleation theory, two-step nucleation, or the pre-nucleation cluster pathway [2,3].
In this context, we examine the nucleation of trisilver citrate crystals using potentiometric titrations and subsequently transfer the solid sample into a porous silver matrix by applying different heating temperatures. The accessible surface areas for silver nanoparticles, whether porous or not, are typically limited to a few square meters per gram. We also test our hypothesis that porous silver can be obtained through the thermal decomposition of solid silver citrate precursors. We conduct a systematic investigation into the formation of silver with high surface areas from both crystalline and amorphous silver citrate.

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Modern Software Techniques for Fast-Fourier Transforms (FFTs) on Today's High Performance Computing (HPC) Architectures

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Plane-wave DFT calculations rely on the efficient and scalable execution of large numbers of 3D-FFTs. However, due to the low computational intensity of FFTs (NlogN operations on N data points), this is an increasing challenge on today's HPC systems. To be able to make use of many compute nodes with their ever-increasing number of cores, new algorithms for data distribution and communication in 3D-FFTs are required. To achieve this goal, we have applied several modern code optimization strategies to enhance the FFT library used by the AIMD code openCPMD. Data locality is exploited by the introduction of shared memory windows. Overlapping computation and communication, batching of messages, and auto tuning algorithms are introduced. The OpenMP parallelization is revised to allow complementary use of MPI and OpenMP for a flexible adaptation to future HPC architectures. The increased node-level performance and scalability across nodes is demonstrated by a series of benchmark calculations.

Optimizing Parameters in Metadynamics Simulations for Free Energy Calculations

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The calculation of free-energy surfaces (FES) is essential for understanding chemical reactions. Especially the free-energy differences between educts, products and possible transition states (reaction energy and activation barrier), allow insight into their nature. Well-sliced metadynamics (WS-MTD) [1] is a novel method to calculate FES by combining umbrella sampling and metadynamics. However, it employs several fine-tuning parameters whose exact influence on the efficiency and accuracy is not yet well understood. In this study, the FES of the reaction of 1,3-butadiene and ethylene to cyclohexene was calculated by WS-MTD. This reaction is well studied and could be used as benchmark to compare the influence of the studied parameters. Using FES calculated with different values of the relevant parameters, the activation barriers and reaction energies were determined and compared to literature values.

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Solution-based Atomic Layer Deposition of Copper: Process Development, Surface Chemistry, and Film Quality Optimization.

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Atomic layer deposition (ALD) is a well-established technique for fabricating thin films with atomic precision. Solution-based ALD (sALD) offers a cost-effective, low-temperature alternative using liquid precursors and solvents. It also expands the variety of precursors applicable to atomic-layer processing significantly. This study provides a case by establishing an sALD process for depositing metallic Cu. Metals have been difficult to access from the gas phase. We exploit the reduction of CuSO4 with ascorbic acid to deposit metallic copper on oxidic and metallic substrates. We explore process parameters, demonstrate self-limiting surface chemistry of deposition, characterize the films, and optimize the film quality.We identify nucleation and solvent purity as the most crucial challenges affecting the film quality. Surface pretreatment allow us to achieve high nucleation density and continuous films of limited roughness.

Characterization of FcgRIV+ B cells in metastasis

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Tumours are structures with a unique microenvironment. Dependent on the kind of tumour and the location, different cell types play a critical role in tumour growth or suppression. While the role of some immune cells has been well studied, B cells have been mostly overlooked. B cells are the antibody producing part of our immune system and are thus mainly regarded as immune system activators [1].
Tumour experiments revealed a to this date unknown inhibitory B cell subset with a specific antibody-binding receptor. It is very surprising that B cells express this receptor as they produce antibodies and could therefore self-activate through binding.
We found that these B cells are present in different organs. Upon tumour growth, these cells seem to travel into the side of metastasis, where they may interact with tumour cells or other immune cells. Modulation of those B cells could thus be used to alter tumour growth.

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Engineering the Chemistry in the Confined Space of 2D Heterostructures

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This project aims to identify functionalization strategies for achieving covalent patterning of 2D surfaces and methods for fabricating 2D heterostructures. Covalent heterostructures address the limitations of van der Waals interfaces by providing improved stability, stronger bonding, and precise functionalization, unlocking advanced applications in energy, catalysis, and electronics.
Building on our previous research, covalently coupled heterostructures can be constructed by connecting molecular linkers attached to functional domains of the bottom layer (MX_2) with the top material layer (Graphene or $M'X'_2$).
We have designed and synthesized three types of molecular linkers: 4′-Bromo[1,1′-biphenyl]-4-diazonium salt, 4-[2-(4-bromophenyl)ethynyl]benzenediazonium salt, and 4-bromo-[p-Terphenyl]-4′-diazonium salt, each optimized to provide specific interlayer spacing.
Covalently functionalized bottom layers were fabricated and analyzed using Raman spectroscopy, photoluminescence (PL), atomic force microscopy (AFM), and X-ray photoelectron spectroscopy (XPS). This study provides the synthesis of three new diazonium salts, which are covalently linked to the bottom layer of 2D heterostructures, offering insights into the optical and electronic properties of 2D materials.

Conventional Hydrogels effect the morphology and fate determination of glioblastoma cell lines in 3D

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3D cell culture models represent cell extracellular matrix (ECM) interactions more accurately than 2D cultures, providing insights into proliferation, adhesion and migration [1]. Two glioblastoma cell lines (U87-MG, LN18) were cultured in five hydrogels: collagen, Matrigel, alginate, oxidized alginate–gelatin and thiolated hyaluronic acid. Cyclic compression tests of the pure hydrogels showed shear moduli of 30–110 Pa, comparable to native human brain tissue [2]. However, cells in collagen and Matrigel adopted astrocytic-like shapes with protrusions versus rounded, spheroid-like cells in the remaining hydrogels. Fractions of cells committed to apoptosis due to ECM detachment as well as to senescence with increased expression of inflammatory cytokines. To improve physiological relevance, we aim to expand hydrogel complexity with brain-specific proteins or lipids and by co-culturing with neurons, astrocytes, or microglia [3].

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Bacterial Nanocellulose as a Matrix for Controllable Liposome Mediated Drug Release

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The renewable biopolymer bacterial nanocellulose (BNC) is a promising material in wound dressings, tissue engineering, and drug delivery. Since it consists of > 90% water, for the incorporation of lipophilic drugs in the nanocellulose matrix sophisticated strategies are necessary [1, 2]. In the present study, liposomes loaded with the lipophilic drug coenzyme Q10 were integrated into the BNC network to control drug and liposome loading and release. Systematic variation of parameters such as phospholipid content and additional surfactant types and concentrations as well as release conditions enabled the establishment of structure-activity relationships (SAR). Those parameters were identified that are critical for the release of drug and liposomes.
Conclusively, the SAR enabled the formulation of delivery systems with controllable release of drug and liposomes from the BNC matrix.

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Archaeal Tetraether Lipid Derivatives to Unlock Efficient Oral mRNA Delivery

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Tetraether Lipids (TELs) empower archaea to live under most extreme conditions due to their unique physicochemical properties: Their ether bonds can withstand low pH values, enzymes, and high temperature, making them a promising candidate to enable oral application [1]. Here, the TEL glycerol dialkyl glycerol tetraether (GDGT) from *Picrophilus oshimae* with modified head groups is investigated for its efficiency in mRNA delivery.
Various GDGTs, functionalized with different ionizable/cationic head groups, were used to prepare mRNA-loaded archaeosomes by ethanol injection method. Dynamic light scattering measurements demonstrated suitable and stable size characteristics. All archaeosomes showed a successful and high mRNA binding as assessed by fluorescence-based measurements. Additionally, a high *in vitro* performance could be observed regarding the transfection efficiency with mRNA encoding the green fluorescence protein.
Based on these findings, these archaeosomes could be suitable candidates for the oral delivery of mRNA.

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Controlling Aggregation-Induced Emission by Sterics in Nitrogen-Boron-Nitrogen (NBN)-Doped Tetraphenylethylene-Like Molecular Propellers

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The phenomenon of aggregation-induced emission (AIE) provides a powerful platform for controlling, boosting and harnessing emission properties in luminescent materials. Here, we report nitrogen–boron–nitrogen (NBN)-substituted molecular propellers derived from tetraphenylethylene with different degrees of steric hindrance. Photoluminescence measurements confirmed AIE behavior in THF/water mixtures for each compound, while the less sterically hindered derivative was characterized by higher emission enhancement due to a more pronounced restriction of intramolecular rotations. A less common maximum behavior was observed upon further addition of water and the effect was found to be more pronounced for the more hindered derivative. Steric hindrance thus serves as effective design tool for enhancing maximum AIE behavior in molecular propellers and achieving more precise control over their photoluminescent properties.

Cellular acute myeloid leukemia (AML) model for preclinical testing of ROS-sensitive prodrugs

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Chemotherapy remains a widespread approach towards cancer treatment but is associated with severe side effects, resulting in approximately every fifth patient developing secondary cancer after treatment.[1] Acute myeloid leukemia (AML) is a particular challenge due to its rapid progression and poor diagnosis, even after intensive chemotherapy.[2] To improve preclinical evaluation of potential anticancer agents, it is crucial to compare their effects on normal and cancerous cells originating from the same tissue. In this study, we used THP-1 cells, derived from a 5-year-old AML-M5 patient, to differentiate them and have a model system for leukemia-like and normal cells. Both cell types were thoroughly characterized, and the effect of different ROS-sensitive anti-cancer agents was systematically investigated and compared. This approach offers a reliable and ethically favorable method while avoiding the need for primary cells and animal models until crucial.

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When Extracellular Vesicles meet Cardenolides: Click Chemistry for Targeted Therapy in non-small cell lung cancer

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Targeted therapies are essential to combat cancer, one of today's leading causes of mortality. A promising approach involves drug delivery via cell-derived extracellular vesicles (EVs). These nanocarriers show biocompatibility and the ability to cross biological barriers [1]. In specific cancers, including non-small cell lung cancer (NSCLC) such as A549 cells, the sodium-potassium ATPase α-subunit is overexpressed compared to healthy cells, making it a potential therapeutic target [2]. Cardenolides are known to bind and inhibit this enzyme. To enhance selective uptake, EV were chemically modified with a cardenolide derivative using a copper-catalyzed azide-alkyne cycloaddition which is more commonly known as click reaction [3,4]. *In vitro* evaluation of A549 cells show decreased cell viability compared to free doxorubicin, demonstrating improved intracellular delivery.

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Controlling molecular motion in azobenzene based molecular brakes and hemithioindigo-based macrocyclic molecular motors with light

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We present two approaches to achieve high level control over molecular motion for light-driven molecular machines and elucidate their working principles with a combination of theoretical and VT-NMR methods.
First, we show that azotriptycenes can serve as a structural framework for photoswitchable molecular brakes. Upon *cis/trans* isomerization, C-N bond rotation rates can be reversibly decelerated or accelerated by up to five orders of magnitude.
Second, we demonstrate how the unidirectional rotation around a dedicated chemical bond can be reprogrammed into unidirectional rotation around a virtual axis. A classical hemithioindigo molecular motor is restricted by macrocyclization, and its intrinsic directional rotation around the C=C bond is transformed into a directional rotation of the macrocyclic chain in the opposite direction.

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Myxobacterial OMVs loaded hydrogels inhibit bacterial proliferation

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In the era of the antibacterial resistance, there is an urgent need for novel compounds and strategies to treat bacterial infection. Outer membrane vesicles (OMVs) released by non-pathogenic myxobacteria have been shown to inhibit both planktonic bacterial growth and biofilm formation[1], highlighting their potential for treatment of wound infections. Designing an appropriate dosage form is pivotal for maximizing their therapeutic efficacy. To this end we propose the use of biocompatible alginate dialdehyde/gelatine (ADA-GEL) hydrogels[2] as scaffold for the release of antibacterial OMVs. Myxobacterial OMVs were successfully incorporated into ADA-GEL hydrogels, which were then characterized in terms of swelling and degradation behavior in different buffers. Furthermore, their ability to release OMVs with retained antibacterial ability have been demonstrated against the model bacteria *E.coli* TG1.

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Magnetic Supraparticles as Identifiers in Single-Layer Lithium-Ion Battery Pouch Cells

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Developing effective recycling technologies is essential for recovering raw materials from lithium-ion batteries (LIBs). Future recycling demands accessible information, supported by digital battery passports connected to physically attached, machine-readable identifiers. Magnetic supraparticles (SPs) offer an innovative solution for labeling opaque materials like battery cells. This contribution demonstrates that SPs with unique magnetic signals can enable rapid, contactless identification of LIB pouch cells *via* magnetic particle spectroscopy (MPS). Therefore, magnetic SPs represent a complementary identification technology for currently employed tags such as QR codes, with the potential to facilitate battery recycling and promote a more sustainable future.

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Physicochemical Studies of Aminoferrocenes as Efficient ROS-Initiators for Targeted Cancer Therapy

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Aminoferrocenes (AFs) are a promising class of redox-active species known for efficiently initiating reactive oxygen species (ROS) production [1]. Their AF-based prodrugs can be selectively activated by H_2O_2, leading to the release of the parent drug in cancer cells and enabling iron-catalyzed ROS generation for targeted cytotoxicity. While the activation mechanisms of AF-prodrugs have been extensively studied [2], the properties of the released AFs under physiological conditions are less understood. In this study, secondary and tertiary aminoferrocenes were synthesized, and their chemical and physicochemical characteristics – including redox potential, catalytic activity, and stability – were investigated under physiological conditions. Optimized synthetic strategies yielded fully characterized compounds, and comparative studies focused on correlating structural motifs with catalytic activity. Planned biological evaluations will clarify the relationship between structural features and cytotoxic effects, confirming the mode of action and highlighting the anticancer potential of these derivatives.

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Tuning the Energy Release in Molecular Solar Thermals via Substituent Position and Autocatalytic Switching

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Molecular solar thermals (MOST) store solar energy in a unimolecular reaction, enabling efficient conversion and storage [1,2]. Electrochemical triggers are promising for energy release due to their precision and reversibility [3]. The electrochemical behavior strongly depends on electron-donating groups in push–pull systems, which allow the absorption spectrum to be better matched to the solar spectrum [4]. Here, we investigate the MOST system methoxyphenylbicyclo[2.2.1]hepta-2,5-diene-2-carbonitrile using in-situ photoelectrochemical IR spectroscopy (PEC-IRRAS), systematically varying the position of the –OMe functionality in the donor group. Ortho and para substitution give highest selectivity (≥98.8%), but differ in onset potentials by 0.3 V_{fc}. An autocatalytic mechanism makes it possible to use the lower onset potential of the ortho isomer to trigger switching in the para isomer. This strategy enables controlled energy release in complex MOST mixtures.

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Hexabenzocoronene-Benzimidazole Hybrid Architectures and Faraday Rotation of Hexabenzocoronene-Phthalocyanine

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The synthesis of three hexa-*peri*-hexabenzocoronene (HBC) derivatives **2-4** including benzimidazole moieties and one tetra-HBC Ni-phthalocyanine (Pc) hybrid molecule **1** is demonstrated. The systems were characterized by NMR techniques, mass spectrometry, UV-vis and fluorescence spectroscopy; they show high molar absorption coefficients throughout with a slight bathochromic shift of the HBC absorption, while molecules **2** and **3** exhibit fluorescence as well. Electrochemical measurements supported by DFT calculations elucidated the electronic structure of the molecules together with excited state molecular orbital analysis using TDDFT. Finally, HBC-Pc **1** was investigated for its ability as a Faraday rotator where it displayed a remarkable Verdet constant of 1.4×10^5 deg $T^{-1}m^{-1}$ at 700 nm in the Faraday A-term.

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Rational Design of Perylene-Rhodium Photocatalysts: A Computational Investigation

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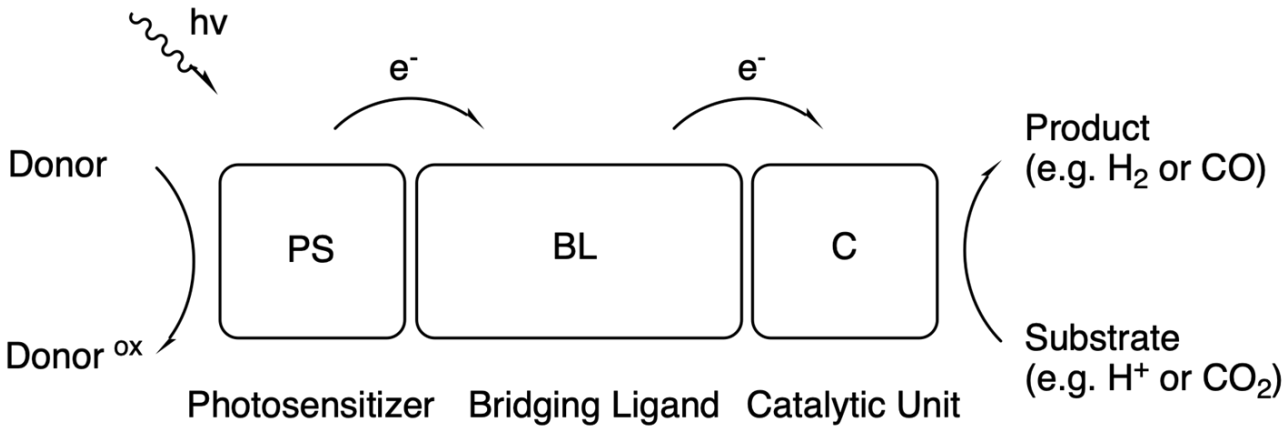
Intramolecular photocatalytic systems, in which photosensitizing and catalytic unit are chemically linked via a molecular bridge, offer a promising approach for light-driven hydrogen evolution reaction, i.e., to generate hydrogen from protons. Efficient photocatalysts demand synergistic connection between the individual components, which can be realized by tuning the electronic properties of the bridging moiety using suitable substituents. Here, these effects are studied within perylene-rhodium dyads ([(phenPer)Rh(Cp+)Cl]).
We investigate how the connectivity between the photosensitizer and bridging unit governs the photophysical properties of intramolecular photocatalysts in two redox states of the rhodium center, Rh(III) and Rh(I). Conformational minima were optimized on the ground (S_0) and triplet (T_1) potential energy surfaces using DFT, providing the basis for simulating transient absorption spectra from direct $S_0 \rightarrow T_1$ excitation. This analysis reveals how excited-state character and charge redistribution depend on both redox state and molecular conformation. Electron-withdrawing substituents red-shift the Rh(III) → Rh(I) reduction, while dihedral flexibility strongly modulates excited-state absorption intensities, highlighting the conformation-dependent tunability of these photocatalysts.



Modulation of tumor-associated macrophages via the FcgRs

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Macrophages are specialized phagocytic cells that are present in all tissues. They engulf and digest pathogens, infected or dying cells, and debris. In addition to this direct function, macrophages can recruit and regulate other immune cells and aid in tissue repair. Nevertheless, in the event of a disease such as cancer, these functions undergo changes. In the context of tumor and metastasis development, macrophages are classified as tumor-associated macrophages (TAMs). These macrophages exhibit either pro-tumor or anti-tumor functions.
Our research aims to identify the function of different TAM subsets in the development of lung metastasis. To facilitate this process, mice were intravenously injected with B16F10 cells, which led to the formation of pseudo-metastasis in the lung. Furthermore, we are evaluating the nasal administration of a therapeutic antibody. This treatment is suitable for reducing metastasis load in mice, and alters the abundance of the TAMs in the lung.

Stress-induced potato yield loss is mitigated by the overexpression of the tuber-inducing gene SP6A at the cost of defense

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Potatoes (*Solanum tuberosum* L.) are a global staple crop, providing starch, amino acids, and vitamins. Tubers develop in response to endogenous and environmental signals. Heat has a negative impact on tuberization; therefore global warming poses a risk to potato yields and food security. Breeding efforts have yet been unsuccessful to overcome this susceptibility.
Our experiments revealed that nitrogen fertilization worsens heat-mediated yield losses. To overcome these limitations, we overexpressed SP6A (SELF-PRUNING 6a). SP6A functions as a mobile signal inducing tuber formation. This overexpression (OE) increased tuber yields across various conditions. Strikingly, SP6A-OE plants utilized high nitrogen to further increase tuber weight instead of shoot growth.
RNA analyses showed that SP6A-OE downregulates defense pathways, and reduces contents of secondary metabolites, consistent with higher potential pest susceptibility. We hypothesize that the increase in tuber yield in SP6A-OE plants results from reallocating resources away from defense metabolism.
Despite a reduced immune response, modulation of SP6A offers a promising approach for ensuring future food security in a changing world.

Enhancing Flexibility of Personalized Formulations: Replacement Strategies for Emulsifiers in a Compounded Semi-Solid Preparation

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Compounded preparations provide an indispensable complement when licensed medicines are lacking. Drug shortages, dosage or formulation adjustments, and allergies require patient-specific preparations [1]. Therefore, standard pharmaceutical base creams require adaptations to ensure timely supply. This study evaluated alternatives for the emulsifier system of the nonionic hydrophilic cream within structurally related components while maintaining stability and physicochemical properties.

Variation of the fatty alcohol chain length and molar mass of the emulsifier polyoxyl 20 cetostearyl ether resulted in formulations with comparable appearance, applicability (sensory, spreadability), and texture (penetration depth, viscoelasticity). Only minor variabilities in the shortest chain-based cream's remaining visual and haptical properties were observed. Reducing the co-emulsifier cetearyl alcohol to its individual components produced unstable formulations. For a shorter-chained co-emulsifier, stability of the cream could be restored by molar-equivalent concentration adjustment.

In conclusion, the emulsifier can be replaced by structurally related components, while changes in the co-emulsifier critically affect the formulation's stability and may require concentration adjustment.

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