GDCh JCF

FJS 2026

COLOURFUL CHEMISTRY

Spring Symposium 2026

10th –13th of March in Cologne



KÖLN LEVERKUSEN JCF

GDCh JCF DÜSSELDORF

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Greetings from Tobias A. Behn, Pia Heinrichs and Leon Bardhi
Heads of Conference Spring Symposium 2026 Cologne

Dear participants,

It is a great joy and an honour to welcome you to the 28th Spring Symposium of the Young Chemists Network (JCF), the FJS 2026, here in Cologne.

This year, we have chosen the theme „Colourful Chemistry", which we mean in every sense of the word. Chemistry is not monochromatic. It is a discipline painted in a thousand hues, spanning diverse research fields and methodologies, and defined by the remarkable diversity of the people who dedicate their curiosity and passion to it. Early-career researchers and senior scientists, theoreticians and experimentalists, specialists and generalists collectively shape a community that surpasses the sum of its parts.

There is no other city in Germany that embodies this spirit as Cologne does. This city is world-renowned for its Carnival, a festival that each year brings together people from all social and cultural backgrounds. Carnival does not sort or exclude, it invites everyone to be themselves and express themselves, to celebrate together, and to leave behind perceived boundaries that so often divide us in everyday life. With a culture of openness, joy and diversity, it reflects core principles that we believe should also be embraced by the scientific community.

With „Colourful Chemistry", we want to move beyond simply acknowledging diversity, but celebrate it. The different backgrounds, perspectives, life experiences and disciplines that scientists bring to chemistry are not a challenge to be overcome, but our greatest asset. The most transformative ideas often emerge at the interfaces between fields and across borders, where complementary expertise and diverse perspectives meet. We want this symposium to be a space where every voice is heard, where different paths into chemistry are recognised as equally valued, and our discipline can emerge in all its colours.

This spirit is reflected throughout the scientific programme. Our speakers embody the colourful breadth of modern chemistry, presenting unique approaches that illuminate their respective field from unexpected angles. From fundamental research to applied science, from materials to life sciences, the range of topics on stage this year is as vibrant as the theme suggests. We are especially proud to present early-career researchers who share their new visions for their fields, representing the next generation of scientists actively shaping the future of chemistry.

We sincerely thank everyone who made this symposium possible. Special thanks to the four JCF regional groups, the GDCh, all our sponsors, and to the University of Cologne. Above all, we thank you, the participants, for bringing your colour to our community and our symposium.



Greetings from Lena Bonitz
Chair of the Young Chemists Network (JCF)



Dear colleagues, dear friends,

A very warm welcome to **Cologne**! On behalf of the National Board of the Young Chemists Network (JCF), I am thrilled to see our community gathered here for this year's **Spring Symposium**. We, as the JCF, are proud to host this event, bringing together young researchers from diverse fields and backgrounds to exchange ideas, foster collaboration, and celebrate the vibrancy of our science.

This year's theme, **„Colourful Chemistry,"** perfectly captures the essence of our discipline. Chemistry is far from monochromatic; it is a vast and brilliant spectrum of research. From the intricate niches of specialized laboratories to large-scale industrial applications, the sheer variety of topics and people present here is a testament to the diversity of our community. While we all „do chemistry" in our own unique is the shared passion for science that acts as the white light combining all our individual shades into one powerful beam.

For me, being here in person is always a meaningful experience. Throughout the year, much of our work, whether within the National Board or across our various JCF teams, takes place in the digital sphere. We spend many hours in online meetings and virtual collaborations to move our network forward. While these digital connections are vital, it is only here, in the lecture halls and corridors of a symposium, that the true spirit of the JCF comes to life. Seeing the faces behind the screens and feeling the collective energy of our members is what makes this event a true highlight.

I encourage you to dive headfirst into this coloruful programme. Step outside your comfort zone, engage with topics beyond your own expertise, and start conversations with those you've never met. Our science thrives on the intersection of different perspectives, and the collaborations you start here will shape the chemistry of tomorrow.

A thank you to the local organizing team for their commitment and to all of you for bringing your unique perspectives to Cologne. Let's make the most of these days and celebrate the colorful world of chemistry together!



Lena Bonitz
Chair of the Young Chemists Network (JCF)

Programme

	Monday, 09.03	Tuesday, 10.03	Wednesday, 11.03	Thursday, 12.03	Friday, 13.03	
08:00						08:00
09:00			Breakfast Opening Ceremony	Breakfast Student Talks	Breakfast Industry Lecture	09:00
10:00			Keynote Lecture	Keynote Lecture	Keynote Lecture	10:00
11:00			Coffe Break	Coffee Break	Coffee Break	11:00
12:00		Registration	Keynote Lecture Young Investigator	Keynote Lecture Young Investigator	Keynote Lecture Industry Lecture	12:00
13:00	JCF Internal Meeting		Lunch	Lunch	Coffee Break	13:00
14:00		Workshops	Keynote Lecture	Young Investigator	Keynote Lecture	14:00
15:00			Coffee Break Industry Lecture	Industry Lecture Coffee Break Industry Lecture	Closing Ceremony	15:00
16:00			Dinner	3 Minute Thesis Final Snack	Social Activities	16:00
17:00		Welcome Reception	Poster Session I	Poster Session II		17:00
18:00						18:00
19:00			Pub Crawl	Conference Dinner Award Lectures		19:00
20:00						20:00

Stay up to date about the programme in our LineUpr App via the QR code
or this link: https://spring-symposium-2026.lineupr.com/spring-symposium-2026

Tuesday, 10th of March 2026

11:30 – 14:00	Registration (Department of Physics)
14:00 – 17:30	Workshops (Meet at registration desk, then Department of Chemistry) Focus matters: Strategic decision making @ ALTANA Einstieg in Generative KI und KI-Agenten für Labor und Forschung - BAYER Excursion CAVE - Cave Automatic Virtual Environment Excursion Chempark Leverkusen - Currenta The Diversity Catalyst: Accelerating Innovation in Science - Evonik Meet a Scientist - How to Science Communication in e.g. schools Rethinking careers in Chemistry: is founding for me? - KOALA Berufseinstieg - vaa Scientific Publishing with Impact - Wiley-VCH GmbH
17:30 – 19:30	Welcome Reception (Department of Physics)

Wednesday, 11th of March 2026

09:00 – 09:30	Opening Ceremony (Department of Physics, Lecture Hall I)
09:30 – 10:30	Keynote Lecture (Department of Physics, Lecture Hall I) Klaus Müllen - Max Planck Institute for Polymer Research, Mainz „Lessons from a live in chemistry: The Chemistry Got to Be Right“
10:30 – 11:30	Coffee Break (Department of Physics, Catering Area)
11:30 – 12:30	Keynote Lecture (Department of Physics, Lecture Hall I) Claudia Wickleder - University of Siegen „Light, Lamps, Luminescence – From Basic Research to Applications“
12:30 – 13:00	Young Investigator (Department of Physics, Lecture Hall I) Alexander Haseloer - Forschungszentrum Jülich „Production Routes for non-Standard Radionuclides for Nuclear Medical Applications“
13:00 – 14:00	Lunch (Department of Physics, Catering Area)
14:00 – 15:00	Keynote Lecture (Department of Physics, Lecture Hall I) Dibyendu Das - Indian Institute of Science Education and Research „Non-equilibrium self-assembly for living matter-like properties“
15:00 – 15:15	Coffee Break (Department of Physics, Catering Area)
15:15 – 16:30	Industry Lectures (Department of Physics, Lecture Hall I) „Enamine´s advances in accessible chemical space development“ „ALTANA - Why we as chemists should care about strategy development“ „tesa Industry Lecture“ „Sustainable Surfactant Development at Evonik“
16:30 – 17:00	Dinner (Department of Chemistry)
17:00 – 18:30	Poster Session I (Department of Chemistry)
18:30 – open end	Pub Crawl

Thursday, 12th of March 2026

09:00 – 10:00 Student Talks (Department of Physics, Lecture Hall I)

Antonia Rabe - „Development of a drone-based measurement system for real-time monitoring of volcanic gas composition at Etna volcano“

Harrison Toll - „Controlled Synthesis and Design of Highly Multiplexed Upconverting Nanoparticles for Live-Cell Imaging“

Alena Neudert - „Coupling voltametric experiments and kinetic Monte Carlo simulations - Insights into hybrid all-Fe redox flow batteries“

Ahmet Cetinkaya - „Designing Polymeric Adsorbents for Sustainable PFAS Remediation“

Chang-Ki Moon - „Electrochemiluminescence based on the formation of exciplex/excimer“

09:00 – 10:00 Student Talks (Department of Physics, Lecture Hall II)

Durgalakshmi Sivasankar - „Enabling activity-based protein profiling (ABPP) for drugs that form disulfides: identification of off-targets for an ALS drug candidate“

Maximilian Wohlgemuth - „Direct Mechanocatalysis - A novel technique for sustainable Catalysis“

Julius Wiener - „Anomeric Amide-Enabled Alkene-Arene and Alkene-Alkene Aminative Coupling“

Takuma Miyamura - „Spin-State Photoswitching in a [5]Helicene-Based Hydrocarbon“

Margarethe Bödecker - „The HyDRA blind challenge on microhydration: past, present and future“

10:00 – 11:00 Keynote Lecture (Department of Physics, Lecture Hall I)

Michael Hocek - IOCB Prague

„Base-Modified and Hypermodified Nucleic Acids for Chemical Biology“

11:00 – 11:30 Coffee Break (Department of Physics, Catering Area)

11:30 – 12:30 Keynote Lecture (Department of Physics, Lecture Hall I)

André Isaacs - College of the Holy Cross, USA

„Teaching Where Students Are: Authentic Science Communication in Digital Spaces“

(continued on the next page)

Thursday, 12th of March 2026 (continued)

12:30 – 13:00	Young Investigator (Department of Physics, Lecture Hall I) Line Næsborg - University of Münster „On the importance of the reaction medium for photochemical synthesis“
13:00 – 14:00	Diversity Lunch (Department of Physics, Catering Area)
14:00 – 14:30	Young Investigator (Department of Physics, Lecture Hall I) Amina Benchohra - University de Bretagne Occidentale „Tuning the luminescence of Cr(III) organometallic and coordination complexes“
14:30 – 15:00	Industry Lecture (Department of Physics, Lecture Hall I) FACCTs „From Academic Theory to Industrial Practice: Quantum Chemistry with ORCA for Real-World Chemical Applications“
15:00 – 15:15	Coffee Break (Department of Physics, Catering Area)
15:15 – 15:45	Industry Lecture (Department of Physics, Lecture Hall I) Novo Nordisk „Innovations in Peptide Chemistry to Enable Discovery of an Oral, Unimolecular GLP-1 and Amylin Receptor Agonist“
15:45 – 16:15	Student Talks (Department of Physics, Lecture Hall I) Gruppo Giovani - „Connecting Young Chemists: The Role of Società Chimica Italiana“ Alexandra Tietze - „Working Under Pressure: Empirical Findings on the Challenges Facing PhD Students in Chemistry“
16:15 – 16:30	3-Minute Thesis Final (Department of Physics, Lecture Hall I)
16:30 – 17:00	Snacks (Department of Chemistry)
17:00 – 18:30	Poster Session II (Department of Chemistry)
19:00 – 21:00	Conference Dinner (Satory Halls)

Friday, 13th of March 2026

09:30 – 10:00 FAIR4Chem Award (Department of Physics, Lecture Hall I)
Marius M. Engler – „Supplement Data of Anolytes for All-Iron Redox-Flow Batteries“

10:00 – 11:00 Keynote Lecture (Department of Physics, Lecture Hall I)
Mie Andersen - Aarhus University
„Uncovering Molecular Origins in Space with Computational Chemistry and Machine Learning“

11:00 – 11:30 Coffee Break

11:30 – 12:30 Keynote Lecture (Department of Physics, Lecture Hall I)
Joleen Masschelein - Katholieke Universiteit Leuven
„Elucidating And Exploiting Novel Microbial Pathways For Antibiotic Biosynthesis“

12:30 – 13:00 Industry Lecture (Department of Physics, Lecture Hall I)
BAYER – „Discovery of a novel oral NO- and heme-independent sGC activator runcaciguat (BAY 1101042)“

13:00 – 13:30 Lunch

13:30 – 14:30 Keynote Lecture
Caroline Murawski - TU Dresden
„Organic semiconductors for flexible, biomedical devices“
Lecture Hall I - Department Physics

14:30 – 15:00 Closing Ceremony (Department of Physics, Lecture Hall I)

15:15 – 17:30 Social Activities
Brewery Tour, Chocolate Museum, Cologne Cathedral, Cologne City Tour


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The **Spring Symposium 2026 (FJS 2026)** brings together emerging researchers from across Europe and beyond to present and discuss colourful topics in chemistry. The conference offers a comprehensive program that combines scientific exchange with opportunities for networking and professional development.

The core of the symposium consists of the scientific sessions, including not only **keynote lectures** by renowned international scientists but also **young investigator lectures**, where upcoming group leaders can present their work. These sessions are complimented by **student talks** from PhD students, where participants share and discuss their latest research findings in depth. In addition, we have organized two **poster sessions**, designed to facilitate detailed discussions and foster interactions among participants. Last but not least, **Workshops and Excursions** convey valuable insights and softskill development.

Alongside the scientific programme, a variety of social events and opportunities for soft skill development complement the symposium. The **welcome reception**, several **coffee breaks** and the **conference dinner** offer the relaxed, yet valuable opportunity to exchange over food and drinks, sparking interesting conversations.

Complementing this, is the **sticker book** to foster interaction with exhibitors and encourage you to take part in the **pub crawl**. **Social activities** as lively outings take participants on a fun and sociable journey through the city of Cologne and the surrounding area. We aim to celebrate the open and welcoming nature of the Rhineland area, which is also reflected in this year's motto „Colourful Chemistry" and are looking forward to you becoming a part of it!

Student Talks

Next to our plenary speakers, selected participants will present their research in an oral communication during one of the sessions on Thursday from 9:00 to 10:00. The parallel sessions will take place in the lecture halls 1 and 2 of the Department of Physics.

Poster Sessions

Due to popular demand, there will be two poster sessions on Wednesday (poster 1-80) and Thursday (poster 81-160) from 17:00 to 18:30 each. The poster session will be held in the foyer of the Department of Chemistry right across the main conference site. Posters can be put up from 15:00 on Wednesday and Thursday respectively. Posters are kindly requested to be removed by 19:00 on the same day. There are several posterprizes which will be awarded during the closing ceremony on Friday.

Workshops and Excursions

The workshops and excursions by our sponsors and partners are the ideal opportunity for you to get know-how from true professionals in their respective fields! The workshops will take place on Tuesday afternoon. You should have received detailed information about the workshop that you have registered for via e-mail.

Three Minute Thesis Finale

After the big success at the GDCh Science Forum 2023 in Leipzig, the Young Chemists' Network is bringing back the JCF Three Minute Thesis. A competition for young investigators that tests their capabilities for good scientific communication. Last year, regional sections of the JCF were holding their local qualifiers. In these preliminary rounds, contestants distilled their research into just 180 seconds, presenting with a single static slide and no animations. The challenge: make cutting-edge science clear, concise, and accessible beyond disciplinary borders.

Now at the JCF Spring Smyposium, we have invited the winners to return to the stage and present their work. Join us to discover outstanding research, compelling stories, and inspiring examples of how chemistry can be communicated with precision, clarity, and impact.

Welcome Reception

The welcome reception on Tuesday at 17:30 will formally open the symposium. In a relaxed atmosphere you will have the opportunity to exchange ideas in an informal setting over some drinks and snacks.

Diversity Lunch

The diversity lunch on Thursday from 13:00 to 14:00 will be hosted by the Team Equal Opportunities. It provides a space for open discussions on diversity and equal opportunities in science. Grab your lunch, exchange ideas, and connect with like-minded participants.

Conference Dinner

The conference dinner on Thursday, marks the last evening of the conference. We aim to celebrate a successful event with you in one of Colognes most renowned event venues – the Sartory Halls. The doors open at 19:00. At 19:30 we will start the evening with a short welcome and the award ceremony of the NFDI4Chem award. At the subsequent buffet you can indulge in some great food and drinks. After the dinner the evening does not end. So better do not return home early, you might miss some great programme.

Please note that participation requires a registration prior to attending. Your conference badge will serve as a ticket so please make sure to wear it openly during admission.

BASF Coffee Bike

Do not miss the opportunity to connect with other participants over a nice coffee. Thanks to the generous support by BASF the beloved Coffee Bike will supply freshly brewed coffee specialties throughout the conference. It is located at the back of the foyer in the Department of Physics.

Social Activity

Participants can explore Cologne through organized social activities. A guided city tour introduces the historic center and landmarks like the Cologne Cathedral, with optional visits to museums or a brewery tour to taste traditional Kölsch beer.

Sticker Scrapbook Challenge

Take part in our scrapbook challenge: visit company booths to collect stickers and fill your scrapbook. Completed books are used to enter a prize draw announced at the closing ceremony. During the pub crawl, collect stamps at participating bars to earn the official FJS 2026 Bier-Bachelor.

Pub Crawl

Explore the surrounding bars in our Pub Crawl. Pass all the exams for your Kneipen-Bachelor, by visiting the pubs listed in your sticker book and get a stamp from all of them. Once you have a full book, you can officially call yourself a „FJS Kneipen-Bachelor“. Some of the bars also have special offers for you.

Tankstelle

Tankstelle is a cozy, laid-back bar known for its quirky interior, including distinctive seating made from car seats and a relaxed, welcoming atmosphere. It’s a popular meeting spot offering a wide selection of drinks, from local Kölsch beers to Belgian varieties.

Pütz

The PÜTZ brewery is an authentic piece of Cologne! What makes the Pütz brewery so special is that the so-called Schwemme, the Köbesse‘s work area, is located openly in the middle of the restaurant. You literally sit in the bar area and can watch the Köbessen tapping the beer. Experience the unique Veedels brewery culture!

RedFox

RedFox is a retro arcade bar in Cologne Ehrenfeld, that combines the relaxed charm of a local bar with the buzz of a modern city hangout. There you can enjoy classic arcade games like skee-ball, creative drinks, and relaxed music in a playful atmosphere. Discover what makes it truly special: its irresistible blend of retro arcade nostalgia with a cozy, vibrant bar vibe.

Päff

The Päff Bar is located in the heart of Cologne—right in the middle of the Friesenviertel. Here you have the rare opportunity to enjoy fresh Päffgen Kölsch—straight from the brewery next door!

Zum Scheuen Reh

The bar “Zum Scheuen Reh”, located right next to West Station, offers a wide selection of drinks and a large outdoor area. After 10 p.m., the Cologne label SOUND SOUND ensures a great atmosphere at “Zum Scheuen Reh”. Look forward to the finest house grooves!

Woody‘s Saloon

Woody’s Saloon is a lively sports bar in Cologne’s vibrant city center, blending the casual energy of game-day cheers with the warmth of a neighborhood favorite. Similar in spirit to the Red Fox, the bar also offers an expanded range of games, including shuffleboard and mini bowling, adding an extra layer of entertainment to the experience. There you sip refreshing craft beers and cocktails, and savor hearty pub bites amid upbeat tunes and an electric crowd vibe.


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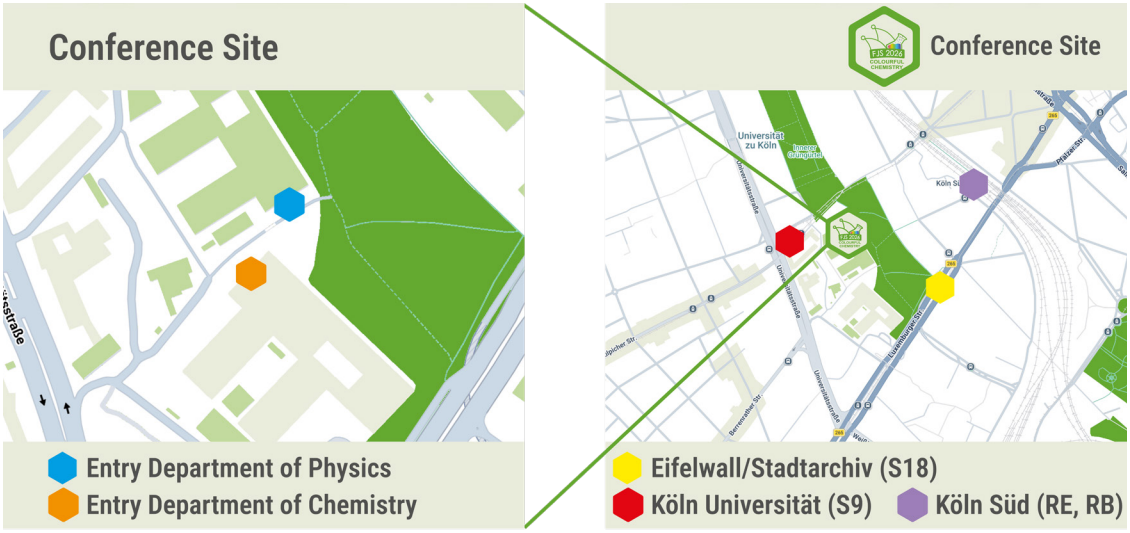
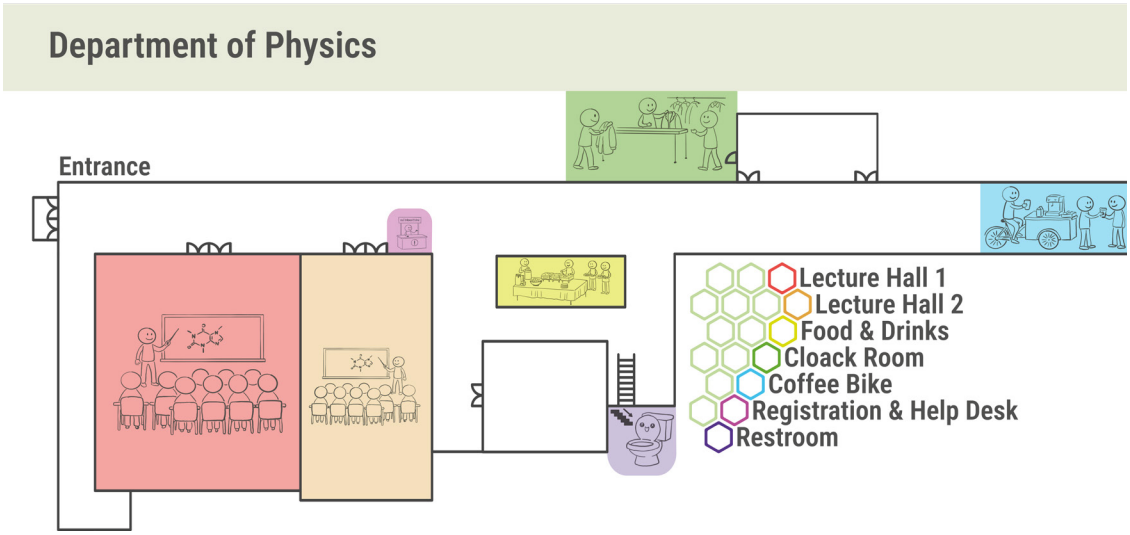
Conference Site

The main part of the scientific program will take place at the **Department of Physics at the University of Cologne (Zülpicher Straße 77, 50937 Cologne)**. This includes the registration, the scientific talks and the lunch breaks as well as the exhibition. The poster sessions will be held at the **Department of Chemistry (Greinstraße 6, 50939 Cologne)**, which is located right across the main conference site.





You can reach the conference site by public transport either via tram line 18 until station Eifelwall/ Stadtarchiv or tram line 9 until station Universität. From there you can walk to the conference site in 5 minutes. Additionally, you can take regional trains (RE5, RE22, RB26 and RB48) from Cologne Central Station until Köln Süd, from where the conference site can be reached in 10 minutes. Furthermore, a nextbike service (KVB-Rad) offers bike sharing for which the nextbike app is required. Bikes can be found through the app in the whole city and be returned in the designated areas. Since parking spaces are extremely limited around the conference site we do not recommend arriving by car.

Conference Dinner

For the conference dinner we will move to the **Sartory Halls (Sartory Säle, Friesenstraße 44-48, 50670 Cologne)**. The Sartory Halls can be reached from the main conference site via a 30 minute walk through Colognes beautiful “green belt” or via tram line 9 or 18 from Universität or Eifelwall/Stadtarchiv, respectively until Neumarkt plus a 10 minute walk.



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Organising an event like the Spring Symposium takes dedication, careful planning, and teamwork. Here, we proudly introduce the hands and brilliant minds driving the operation, the team making everything run smoothly behind the scenes.

Head of Conference







Team Programme









Team Sponsoring & Finance













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Uncovering Molecular Origins in Space with Computational Chemistry and Machine Learning

Dr. Mie Andersen

Aarhus University, Denmark

Complex organic molecules have been found in comets, and molecules such as acetone and dimethyl ether have been detected in the interstellar medium via telescopes. Although their formation pathways remain poorly understood, there is strong evidence that surface reactions at dust grains play a decisive role.

Here I will present the computational methods we use—including ab initio methods such as density functional theory (DFT) and machine learning interatomic potentials (MLIPs)—to model dust grains and their interaction with molecules. Dust grains are mainly composed of abundant elements like C, Si, O and Mg, and we have modelled these using either a thin sheet of C (graphene) or as Mg-rich silicates.

Within dense and cold gas clouds, the grains may be partially or completely covered in ices consisting of abundant interstellar molecules like H_2O, CO_2 or CO.By training MLIPs on DFT data, we can model the structure and dynamics of ice formation on dust grains at near-DFT accuracy, but orders of magnitude lower computational cost. This enables us to probe larger, and hence more relevant, system sizes and timescales in molecular dynamics simulations. I will show how we use these simulations to interpret laboratory experiments on ice growth and to deduce crucial parameters such as binding energies for astrochemical models of the molecular evolution of interstellar gas clouds.

About Dr. Mie Andersen



Associate Professor in the Department of Physics and Astronomy at Aarhus University in Denmark. She received her PhD in Nanoscience in 2014. Subsequently, she held an Alexander von Humboldt postdoctoral fellowship and worked as a group leader at the Technical University of Munich in Germany. She has received several fellow- ships and awards, including a fellowship at the Aarhus Institute of Advanced Studies, a fellowship for distinguished visiting scientists of the Max Planck Society, and the Gerhard Ertl Young Investigator Award for excellence of research in surface science of the German Physical Society. Her current research interests include data-driven materials modelling, heterogeneous catalysis and astrochemistry.

Non-Equilibrium Self-Assembly for Living Matter-Like Properties

Prof. Dr. Dibyendu Das

Insitute of Science Education and Research, India

Life is soft and wet machinery arose from spatially confined assemblies of biomolecules capable of replication, integrated with metabolic reaction cycles that function far from equilibrium. By methodically synthesizing and integrating these key elements, i.e. replication, metabolism, and confinement under non-equilibrium conditions, we can begin to explore how chemically constructed systems might acquire life-like, evolving properties. This ambitious goal lies at the heart of systems chemistry. In this talk, I will outline recent insights into how reaction networks, self-reproduction, and compartmentalization can be brought together under non-equilibrium settings. I will also delve into the interplay between reaction dynamics and transient compartmentalization, and explore the development of self-replicating systems capable of sustained operation in far-from-equilibrium conditions.

About Prof. Dr. Dibyendu Das



Professor at the Department of Chemical Sciences at the Indian Institute of Science Education and Research (IISER) Kolkata, West Bengal in India. He obtained his PhD in supramolecular chemistry at the Indian Association for the Cultivation of Science (IACS) under the supervision of Prof. P. K. Das in 2010. After a postdoctoral stay at the Emory University with Prof. D. Lynn in the US he started at the IISER as assistant professor, and rose through the ranks to become full professor in 2025. His research group is interested in the emerging field of systems chemistry, chemical evolution and peptide nanotechnology.

Base-Modified and Hypermodified Nucleic Acids for Chemical Biology

Prof. Dr. Michal Hocek

Czech Academy of Sciences, Czech Republic

The lecture will summarize recent results of the Hocek group in enzymatic syntheses of base-modified and hypermodified nucleic acids (DNA, RNA or XNA) and their applications in chemical biology, bioanalysis or imaging. Enzymatic methods for construction of nucleic acids with sequence-specific display of diverse substituents or molecules, as well as hypermodified nucleic acids composed entirely from modified nucleotides will be discussed in detail. Special focus will be given to the use of modified nucleotides in selection of aptamers.

About Prof. Dr. Michal Hocek



Distinguished chair group leader at the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Science (IOCB) and a full professor at the Charles University in Prague. He graduated from the University of Chemistry and Technology Prague in 1993 and finished his PhD at the IOCB in 1996. After a postdoctoral stay at the Université Catholique de Louvain, he joined the IOCB and started his own research group in 2003. He received numerous awards, including the Praemium Academiae from the Czech Academy of Sciences and the R. Lukes Prize from the Czech Chemical Society. His research interests include organic synthesis, chemical biology, as well as medicinal, bioorganic, and nucleic acid chemistry.

Teaching Where Students Are: Authentic Science Communication in Digital Spaces

Dr. André Isaacs

College of the Holy Cross, United States of America

Broadening participation in STEM requires a multipronged approach that acknowledges generational differences in how students learn and engage with the world. For Gen-Z students, social media is not just entertainment but a primary space for cultural exchange, identity formation, and engagement with social concerns. Leveraging these platforms offers unique opportunities to communicate scientific concepts both formally and informally. This lecture will explore strategies for creating effective science communication videos while emphasizing the importance of authenticity. By bringing one's full self—personal identity, values, and lived experiences—into the act of teaching and communication, educators and scientists can foster deeper connections, build trust, and make science more accessible and inclusive. I will showcase my work on social media as a case study for integrating identity and culture in STEM.

About Prof. Dr. André Isaacs



A native of Jamaica, André moved to the US to attend the College of the Holy Cross where he received his B.A. in Chemistry in 2005. He received his PhD from the University of Pennsylvania in 2011 under the guidance of Prof. Winkler. After a postdoctoral stay at the University of California with Prof. Sarpong, he accepted a tenure-track position at the College of the Holy Cross in 2012. Here, he was promoted to the rank of Associate Professor with tenure. Here, he teaches courses in Organic Chemistry and performs his independent research on utilizing copper- mediated organic transformations. André uses his social media platform to challenge and dis- mantle the normative culture in STEM and to increase visibility of queer and BIPOC folks.

Elucidating And Exploiting Novel Microbial Pathways For Antibiotic Biosynthesis

Dr. Joleen Masschelein

Katholieke Universiteit Leuven, Belgium

Microorganisms produce diverse specialized metabolites with important applications in medicine and agriculture. Many clinically relevant compounds are assembled by modular polyketide synthase (PKS) assembly lines, which build complex carbon skeletons from simple acyl thioester precursors through iterative condensation and tailoring reactions. PKS pathways exhibit striking architectural diversity and often involve non-canonical enzymes and unusual catalytic chemistries, making them valuable sources of both novel drug leads and new enzymatic transformations.

To uncover previously unknown biosynthetic mechanisms, we developed genome mining strategies targeting pathways that catalyse unprecedented reactions. This led to the discovery of new anticancer and antibiotic compounds and revealed novel enzymatic transformations, including oxime formation, diene isomerization and unusual chain-release mechanisms. Combining bioinformatics, mutagenesis, chemical synthesis, in vitro assays and mass spectrometry, we elucidated enzyme activity and selectivity. These insights enabled the rational engineering of new polyketide scaffolds. Using mutagenesis, gene deletion and precursor-directed biosynthesis, we reprogrammed microbial systems to produce novel analogues with improved activity and stability, highlighting microbial biosynthesis as a powerful platform for drug discovery.

About Dr. Joleen Masschelein



Associate Professor at the Katholieke Universiteit Leuven. She obtained her PhD in 2015 under the guidance of Prof. Lavigne, Chris Michiels and Abram Aertsen at KU Leuven. Subsequently, she was awarded a Marie-Sklodowska Curie Individual Fellowship to join the group of Prof. Challis at the University of Warwick. In 2017, she performed postdoctoral research at the KU Leuven. After that she was appointed as an assistant professor and promoted in 2025. She received several fellowships and awards, among which the EFMC Prize for a young Chemical Biologist/Medicinal Chemist in Academia.

Her research focuses on the interface between chemistry and biology and targets microbial natural products with potential pharmaceutical applications.

Organic Semiconductors for Flexible, Biomedical Devices

Prof. Dr. Caroline Murawski

Dresden University of Technology, Germany

Kurt Schwabe Institute for Sensor Technologies, Germany

Organic electronics have major advantages compared to inorganic electronics in applications that require mechanical flexibility, patterning to specific shapes, and tunability of device properties. These benefits are particularly interesting in biomedical applications such as wearable and implantable sensors for tracking body functions and manipulating cellular activity.

Here, I will present the development of organic LEDs (OLEDs) and photodiodes (OPDs) as light sources and sensors for biomedical applications. The OLEDs are based on fluorescent, phosphorescent, and TADF emitters, which are selected with specific focus on high power output at low voltages. The emission spectra and angular intensity profiles are tailored using optical simulations. Devices are fabricated on flexible, water-proof substrates, patterned to sub-mm scale, and applied in optogenetics and fluorescence imaging as well as photoplethysmography at ambient light conditions and under water. This work presents major contributions towards engineering wearable and implantable optical devices for sensing and light-based therapy, which ultimately will advance the understanding and treatment of neurodegenerative diseases.

About Prof. Dr. Caroline Murawski



Professor for biomedical sensor technology at Dresden University of Technology. She received a PhD in Physics working on excitonic processes in organic light-emitting diodes in 2015. Then she joined the University of St Andrews as a postodctoral fellow and Marie Skłodowska Curie fellow. In 2018, she started a junior research group at the Kurt Schwable Institute for Sensor Technologies in Waldheim. In 2023 Prof. Murawski transferred to the Dresden University of Technology as young investigator, before she got appointed as full professor and chair for Biomedical Sensor Technology in 2024. Her research revolves around new biomedical sensor technology based on organic semiconducting materials.

Lessons from a live in chemistry: The Chemistry Got to Be Right

Prof. Em. Klaus Müllen

Max-Planck-Institut für Polymerforschung, Germany

In this lecture Klaus Müllen will combine questions of scientific excellence and career choices with key moments from his academic career. Klaus Müllen was born in 1947 in Cologne. He studied chemistry there and obtained his PhD in 1971 at the University of Basel, followed by postdoctoral work and habilitation at ETH Zurich, before holding professorships in Cologne and Mainz and later serving as director at the Max Planck Institute for Polymer Research. Against this biographical backdrop, the talk will explore how organic synthesis and related fields such as polymer and supramolecular chemistry can serve as a platform for highest scientific achievement. Building on selected anecdotes, the lecture will address whether pure scientific excellence is sufficient to reach one's goals or must be complemented by strategic choices in research topics or institutional moves. Particular attention will be given to the specific conditions of the German academic system and how Müllen navigated them transitioning from university chairs to a long-term leadership role at a Max Planck institute. Central to the narrative are the "tipping points" of his career: decisions on scientific direction and institutional opportunities that transformed strong potential into a state where "everything achievable".

About Prof. Em. Klaus Müllen



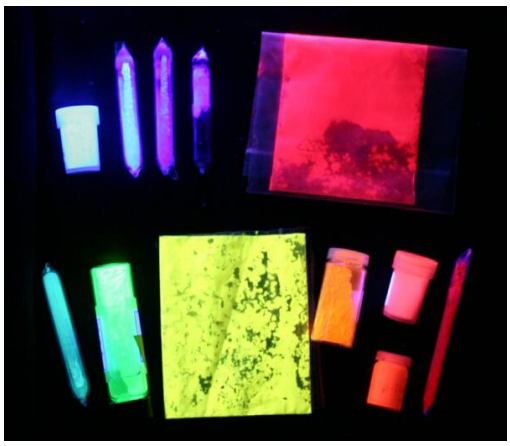
Emeritus director at the Max-Planck-Institut für Polymerforschung in Mainz. He studied chemistry in Cologne and obtained his PhD at the University of Basel under the supervision of Prof. Gerson. After a postdoctoral stay with Prof. Oth at ETH Zürich, he became a professor for organic chemistry at the University of Cologne in 1979 and subsequently at the Johannes Gutenberg- Universität Mainz in 1983. At the Max-Planck- Institut für Polymerforschnug, he headed the Department of Synthetic Chemistry. He has received numerous awards, including the Karl-Ziegler-Preis and the Cothenius-Medaille. His independent work is focused on graphene and graphene nanoribbons and their potential application in information and energy technology.

Light, Lamps, Luminescence – From Basic Research to Applications

Prof. Dr. Claudia Wickleder

University of Siegen, Germany

The development of novel light emitting materials is currently a hot research topic, applications are for instance light emitting diodes (LEDs), solar cells, sensors and security phosphors. In this talk the compounds resulted from our research will be presented after a general introduction of luminescent materials. Furthermore, for all applications a small particle size in the nm (10-9 m) range is very promising allowing e.g. the use as medical sensors in mice. With this approach it is possible to develop cancer markers or investigate the toxicity of fine dust. For this goal the development of novel synthesis methods is necessary to yield highly efficient materials. Finally, luminescent micro plastics will be introduced, which can serve as sensors for the toxicity of micro plastics. During my talk the light emission of some efficient materials will be presented.



About Prof. Dr. Claudia Wickleder



Chair of Inorganic Chemistry at the University of Siegen. She studied chemistry at Hannover University (Diploma, 1981–1989), earned her PhD in Physical Chemistry under Prof. Dr. Hanns von Weyssenhoff (1989–1995), and completed a Postdoc in laser spectroscopy at the University of Bern (1995–1997). She habilitated in Inorganic Chemistry at the University of Cologne (1998–2004) before assuming her current position in 2004.

Her research focuses on luminescent inorganic materials and nanostructures for lighting, sensing, and optical applications. She has extensive international collaborations and has served in leadership roles including Vice Dean and Senate member at Siegen, Vice President of EuCheMS's Division of Inorganic Chemistry, and consultant for numerous national and international funding agencies. She is also active in outreach, coordinating the University of Siegen's Children's University.

Young Investigator Lecture

Tuning the luminescence of Cr(III) organometallic and coordination complexes

Dr. Amina Benchohra

Université de Bretagne Occidentale, France

Over the past decade, the quest of earth-abundant alternatives to the charge-transfer Ru(II) emitters has undoubtedly revitalized chromium(III) chemistry. Their intriguing properties - including a near-infrared (NIR) phosphorescence stemming from metal-centered spin-flip transitions, long-lived excited states (from µs to ms), and efficient sensitization pathways via either ligand-centered (LC), ligand-to-metal charge transfer (LMCT) or metal-centered (MC) excitations- are of interest for photonic devices, photocatalysis or energy conversion. So far, the practical guidelines for optimizing Cr(III) emitters mainly drew on traditional coordination ligands (e.g.: bipyridine, phenantroline and terpyridine derivatives). This talk will describe the design and use of novel series of luminescent Cr(III) complexes relying on contrasted organo-metallic and coordination ligands.

About Dr. Amina Benchohra



Assistant professor at the Université de Bretagne Occidentale in Brest. Following her undergraduate studies at Sorbonne Université, she completed her PhD on the design of switchable hybrid materials based on magnetic molecular complexes under the supervision of Prof. Kreher and Prof. Lescouëzec at the Parisian Institute of Molecular Chemistry in 2019. She then undertook postdoctoral studies on self- assembled materials for solar cells with Dr. Goeb at Moltech-Anjou Laboratory in Angers. After working on the design of Cr(III)-Ln assemblies for energy- transfer upconversion as postdoctoral researcher, and junior lecturer in the group of Prof. Piguet in Geneva, her current research focusses on (multi)- functional molecular materials.

Production Routes for Non-Standard Radionuclides for Nuclear Medical Applications

Dr. Alexander Haseloer

Forschungszentrum Jülich, Germany

In recent years, two very important bioinorganic drugs hit the market, Lutathera and Pluvicto. Both are now the highest grossing metal containing small molecule drugs and have a similar design principle. Basically, it's a biovector, a chelator and a radionuclide – both contain Lu-177. Despite being successful, Lu-177 leaves room for improvement. Mainly its decay radiates further than desired, leading to off target irradiation and side effects.

At the INM-5 we aim to produce radionuclides which have a much smaller penetration depth. For this purpose we develop production routes and chemistry of radionuclides like Pt-193m, Pb-203, and At-211 among others. During this talk I will present our endeavors into the production of these nuclides and their subsequent chemistry.

About Dr. Alexander Haseloer



Junior research group leader in the Institute for Neurosciences and Medicine, Nuclear Chemistry (INM-5) of the Forschungszentrum Jülich. He received his PhD in bioinorganic chemistry under the guidance of Prof. Klein at the University of Cologne in 2021. After that, he moved to Princeton Unitversity as a Walter Benjamin Fellow to learn about photocatalytic method development in the group of Prof. MacMillan. His independent research is focused on the production of non-standard radionuclides and implementing them into the chemistry he learned in his PhD and Postdoc. He was awarded a Liebig Fellowship early 2025.

On the Importance of the Reaction Medium for Photochemical Synthesis

Dr. Line Næsborg

University of Münster, Germany

The reaction medium can be key to induce photochemical reactions. A particular focus is given to aqueous micellar systems to provide unique benefits in photochemistry and photocatalysis. Here, apolar molecules such as oxygen are present in the inner core and charged or polar molecules such as a photocatalyst (PC) can be localized at the interphase. Through preferred localizations, non-productive encounters are minimized and oxygen quenching of a triplet state photocatalyst can be avoided. Based on this, oxygen sensitive photocatalytic reactions could be developed without the need for oxygen removal. However, controlled localization and compartmentalization can lead to further interesting benefits that are important in photochemical synthesis such as enabling complex or excimer formation. For example, we illustrate that a small organic molecule (chalcone) can exhibit excimer emission in the micellar system whereas no such emission could be observed in organic solvents. The phosphorescence was recorded at room temperature and has a surprisingly long average lifetime (19.22 µs). Interestingly photochemical reactivity was accordingly only observed in the micellar reaction medium and not in organic solvent.

The vision of the program is medium-controlled photochemical synthesis that unites physical understanding, reaction design and sustainable implementation.

About Dr. Line Næsborg



Junior research group leader in the Westfälische Wilhelms-Universität Münster. She graduated in medicinal chemistry from the Aarhus University in 2013 and stayed there until 2018 for her PhD studies on the combination of organocatalysis and tran- sition metals in the group of Prof. Jørgensen. After that, she conducted postdoctoral research on photochemical cascades and their application in total synthesis in the group of Prof. Bach at the Technical University of Munich, before she transferred to the WWU in Münster. Her independent research is focused on organic chemistry and photo- catalytic reactions in water to „make the world a little more sustainable through innovative chemistry“.

Discovery of a novel oral NO- and heme-independent sGC activator runcaciguat (BAY 1101042)

Dr. Michael G. Hahn

Bayer AG, Pharmaceuticals, Medicinal Chemistry Wuppertal, German

Soluble guanylate cyclase (sGC) is the intracellular nitric oxide (NO) receptor and plays a key role in a variety of physiological processes such as vasodilatation, antiaggregation, antiproliferation and neuronal signaling. Impairments of the NO-sGC-signaling pathway have been implicated in the pathogenesis of various cardiovascular and other diseases. Current therapies that involve organic nitrates and other NO donors have limitations, including non-specific interactions of NO with various biomolecules and lack of response and the development of tolerance. Consequently, innovative approaches are needed to exploit the full therapeutic potential of the NO/sGC/cGMP-signaling pathway.

Recently, two novel drug classes which activate the soluble guanylate cyclase (sGC) have been discovered. The sGC stimulators (heme-dependent) and sGC activators (heme-independent). sGC stimulators share a dual mode of action, they stimulate sGC directly and enhance sensitivity of sGC to low levels of bioavailable NO. In contrast, sGC activators are able to activate the pathologically changed heme-free sGC. The discovery of sGC activators offered the prime opportunity to design drugs for selective binding to the oxidized, heme free sGC generated by the influence of oxidative stress causally involved in many cardiovascular and cardiorenal diseases. One of the first sGC activators was Cinaciguat [2]. However, this compound was not suitable for oral administration. More recently, runcaciguat a second-generation sGC activator for oral administration has been discovered. The discovery of runcaciguat [3], the structural activity relationship, in vivo results and PoC data in CKD patients will be presented.

About Dr. Michael G. Hahn

Graduated in chemistry and earned a Ph.D. in the Altenbach Group at the University of Wuppertal (1996–1998), followed by postdoctoral research in the Ley Group at the University of Cambridge (1999–2000). Since 2000, he has worked at Bayer Wuppertal in Medicinal Chemistry on programs for heart failure, lung and kidney diseases, and obstructive sleep apnea. He served as responsible & inventive chemist for six clinical candidate nominations since 2011 and received the Global Drug Discovery Award Bayer Pharmaceuticals (2013 & 2015) and the Friedrich-Stolz Award 2022 (GDCh & DPhG) for discovering sGC modulators.

Enamine's advances in accessible chemical space development

Dr. Ivan Kondratov

Enamine Germany GmbH, Frankfurt am Main, Germany

The concept of chemical space is fundamental in the fields of cheminformatics and drug discovery. It can be likened to the cosmos, in that molecules occupy space rather than stars and the whole chemical space refers to the entirety of all possible molecules and known compounds. Drug-like chemical space is extremely vast and is estimated in the region of 10^{63} (molecules considering only the presence of atoms C, N, O, or S, with each molecule having a maximum of 30 atoms) and only a very small part of it (10^{7} molecules) are "off-the-shelf" available from various vendors. In addition the interest to space of synthetically accessible or feasible compounds (which can be made on demand by chemical vendors) is growing during last decades and the importance of such space becomes particularly important due to emerging and growing AI- and computationally driven approaches, which can operate with huge data sets to search for new starting points for drug discovery campaigns.

Enamine is one of the main players and remarkable contributor in this field. The company designs and constantly extends its accessible chemical space using internal tools and technology which allows the company to maintain relatively low costs and high level of synthetic feasibility. Enamine's ultra-large REAL Space of on demand compounds is widely used by numerous researchers worldwide and became a benchmark on the market.

The presentation will cover the topic of development of this accessible chemical space, examples of applications in drug discovery projects as well as approaches used to extend the chemical space and filling the gaps in it.

About Dr. Ivan Kondratov



Master in organic chemistry (2004, Taras Shevchenko National University, Kyiv) and Ph.D. in bioorganic chemistry (2008, V. P. Kukhar Institute of Bioorganic Chemistry NASU, Kyiv). Completed an MBA in Pharma Business Administration at Goethe Business School (2025). Guest scientist at Münster University (2009–2017). Seven years at Enamine Ltd, rising from synthetic chemist to Head of Laboratory, and ten years managing FTE projects. Last five years as Head of Medicinal Chemistry, organizing 40+ customer projects, managing multidisciplinary drug discovery projects, negotiations, and business development. Now at Enamine Germany, building teams and leading MedChem projects.

Bonding for Innovation: From Molecules to Adhesive Tape Solutions

Dr. Thilo Dollase, Yanny Lugemba Budiaki

tesa SE, Hugo-Kirchberg-Straße, 22848 Norderstedt

What happens to chemistry once it leaves the lab - and how does it become a technology used millions of times every day? In this joint industry lecture, tesa offers a behind-the-scenes look at how fundamental chemical research is transformed into high-performance adhesive solutions applied across industries such as electronics, automotive, etc.

The presentation brings together two complementary perspectives. First, tesa will be providing insights into career paths beyond academia, the transition into industrial Technology and Product Development, and opportunities to work at the interface of technology, engineering, and product development. In the second part, it will be illustrated how polymer science is utilized to solve complex technical challenges and deliver market-ready innovations.

About Dr. Thilo Dollase

Graduation from TU Berlin in chemistry including Master Studies in the U.S.A. on liquid crystalline systems. Dissertation work performed at Max-Planck-Institut für Polymerforschung Mainz (“Influence of Rigid Confinements on Local Order and Chain Dynamics in Polymer Melts”) involving a research stay in Israel. Professional career at tesa starting in 2000, having held various positions in R&D in Technology and Product Development as Developer and Laboratory Manager. Since 2020 acting as Senior Scientist for Rubber Technology. Several publications, conference contributions, and numerous patent applications. Soft-matter related 2025 MRS tutorial instructor (“Rubbers and TPEs: Soft but Elastic Materials for Adhesives”).

Sustainable Surfactant Development at Evonik

Dr. Veit G. Hänsch

Evonik Operations GmbH, Rellinghauser Str. 1-11, 45128 Essen, Germany

Evonik is a leading supplier of specialty surfactants and offers a wide range of nonionic, anionic, cationic, and amphoteric surfactants for many industrial and consumer uses. In our development work, we focus on creating high-performance products while making sustainability a key part of our innovation. This includes using renewable raw materials, improving our production processes, and developing surfactants with better environmental profiles. In this process, petrochemical raw materials are being replaced by bio-based or CO_2-based materials. Evonik also uses enzymes in technical scale for selective esterification at low temperatures and produces biosurfactants by microorganisms. With this approach, we help to shape innovative and environmentally friendly products for the future.

About Dr. Veit G. Hänsch



Veit Hänsch received his B.Sc. and M.Sc. in Chemistry from Friedrich Schiller University Jena, including a research stay at McMaster University in Canada. He completed his doctoral research at the Leibniz Institute for Natural Product Research and Infection Biology – Hans Knöll Institute (HKI) in Jena, focusing on photochemistry and total synthesis. He subsequently conducted postdoctoral research in catalysis at MIT in Boston, USA. Since 2025, he has been a Lab Manager at Evonik in Research, Development & Innovation (RD&I) within Care Solutions.

Innovations in Peptide Chemistry to Enable Discovery of an Oral, Unimolecular GLP-1 and Amylin Receptor Agonist

Prof. Dr. Thomas E. Nielsen

Novo Nordisk A/S, Denmark

Late-stage drug discovery often necessitates parallel efforts in both medicinal chemistry and process research to balance the drug-like properties of an API with a viable production path. For peptide and protein drugs in therapeutic areas such as cardiovascular and metabolic diseases, recombinant expression can efficiently and sustainably produce high-volume active pharmaceutical ingredients. However, this approach can also pose challenges to drug design if a range of extensive post-recombinant chemistry is required to preserve drug-like properties. Here, we present a spectacular innovation in process chemistry, a photochemical method to convert recombinantly expressed peptides into biologically active C-terminal α-amides from cysteine-extended precursors. We also describe application of this chemistry, as well as key medicinal chemistry efforts, in the discovery of an oral, unimolecular GLP-1 and amylin receptor agonist.

About Prof. Dr. Thomas E. Nielsen



Vice President of Drug Product Research, Therapeutics Discovery at Novo Nordisk, and affiliated professor at the Department of Immunology and Microbiology, University of Copenhagen. He completed his PhD on natural product total synthesis at the Technical University of Denmark (DTU) under supervision of Prof. Tanner. After that, he performed postdoctoral research in the field of chemical biology at the Carlsberg Laboratory, Harvard University, and the Broad Institute. In 2008, he returned to the DTU as professor of chemical biology before joining Novo Nordisk in 2014. A central theme in his research is the synthesis of small molecules and peptides to probe biology and develop new medicines to treat diabetes, obesity, and many other diseases.

From Academic Theory to Industrial Practice: Quantum Chemistry with ORCA for Real-World Chemical Applications

Christoph Riplinger

FACCTs GmbH, Cologne, Germany

FACCTs operates at the interface of academic quantum chemistry and industrial research, translating modern electronic structure methods into practical tools for chemical problems. This talk introduces the ORCA quantum chemistry program and its application at FACCTs to real-world challenges.

We outline ORCA's scope, from force-field and semi-empirical approaches to density functional theory and correlated wave-function methods, covering molecular properties and reactivity. Quantum-mechanical simulations are combined with experimental techniques such as NMR, IR, Raman, UV/Vis, and chiroptical spectroscopy to support structure elucidation and spectral interpretation, especially when reference data are scarce or spectra are difficult to analyze.

Industrial examples illustrate ORCA-based workflows under realistic constraints, including studies of reaction mechanisms, energetics, selectivity, and molecular recognition. Tools such as ORCA Docker, Solvator, and the conformer search algorithm GOAT enable efficient exploration of potential energy surfaces and identification of relevant conformers and aggregates, bridging academic rigor and industrial application.

We highlight the ORCA Python Interface (OPI), enabling direct control from Python and promoting automation, reproducibility, and data-driven analysis. OPI is also suited for teaching and student projects.

We conclude with perspectives on integrating computational chemistry early in research and on career paths between academia and industry.

About Dr. Christoph Riplinger

Dr. Christoph Riplinger is a trained biochemist (studies in Tübingen, Marseille, and diploma thesis in Cologne). During his academic career with the University of Bonn, the German Max Planck Society and Princeton University he developed quantum chemical methods that allow for an accurate prediction of molecular properties, e.g. the DLPNO-CCSD(T) method, which can be used in combination with, or replace, experimental data. After growing interest in his work from the Pharmaceutical and Chemical industry he co-founded FACCTs GmbH as Managing Director. With FACCTs he now leads the further development of new and ground-breaking predictive methods for Life Science applications, Spectroscopy and Catalysis, with successful collaborations across Pharma, Chemical and Materials Science Industry.

ALTANA Industry Talk: Why we as chemists should care about strategy development

Fabian Stahl

ALTANA AG

The ALTANA Group develops and manufactures high-quality, innovative specialty chemical products. Our four divisions – BYK, ECKART, ELANTAS, and ACTEGA – have set worldwide standards in their markets.

Innovation is ALTANA's growth driver. We create an innovation culture that puts us in a position to make the most of our competencies.

ALTANA expands its product portfolio through own developments, as well as through acquisitions and cooperative ventures with other companies, universities, and scientific institutes.

At ALTANA, innovation is not restricted to research and development but encompasses all processes in the company. Each employee is called upon to seek and realize improvements in their respective area of responsibility. To implement new ideas we take calculated risks. To do so requires courage, the awareness that we may suffer setbacks, and a willingness to take responsibility for mistakes and to learn from them.

Thus, do you still think, chemists do not need to bother about typical topics from business studies like strategy development? We at ALTANA think different: What can we as chemists learn from the process of developing a strategy? By getting to know how ALTANA develops strategies, let us explore what insights we can leverage for university projects, laboratory work and even daily life. Small case studies from the ALTANA universe highlight how relevant it is for an organization to develop the awareness for strategic decision taking.

About



Fabian Stahl is Manger Corporate Strategy at ALTANA. In his role, he supports ALTANA's four divisions developing their strategies and manages cross-divisional projects. Before he joined ALTANA in 2023, he worked for four years at KPMG Cologne as a Strategy Consultant supporting clients from different industries on strategic questions and transactions. Fabian has a M.Sc. in Business Chemistry from University of Münster, a B.Sc. in Applied Chemistry from FH Aachen and worked as a laboratory chemist at Forschungszentrum Jülich for four years

Development of a drone-based measurement system for real-time monitoring of volcanic gas composition at Etna volcano

Antonia Rabe[1],Niklas Karbach[1], Nicole Bobrowski[2,3],Thorsten Hoffmann[1]

[1] *Department of Chemistry, Johannes Gutenberg-University, Mainz, Deutschland*

[2] *University Heidelberg, Heidelberg, Deutschland*

[3] *Instituto Nazionale di Geofisica e Vulcanologia (INGV), Osservatorio Etneo, Catania, Italy*

Volcanic gas emissions provide important insights into magmatic processes beneath the Earth's surface and play a crucial role in assessing volcanic hazards. Depending on their solubility in magma and the respective pressure conditions, volcanic gases are exsolved and released at different depths of a volcanic vent.[1] To study behavior prior to an eruption in hazardous locations, unmanned aerial vehicles (UAVs) offer a safer measurement platform. To increase monitoring frequency, reduce manual labor and the associated risk for the researcher, this work aims to develop a drone station capable of autonomous measurement flights near the volcanic crater.

The sensor system consisting of a SO_2 and CO_2 sensor was developed in-house and can be attached to the drone.[2] To ensure reliable and robust measurement results, a dedicated calibration station was designed and built that allows for easy, repeatable, and automated calibration of the sensor system. The system comprises a pressurized gas container with a calibration gas mixture that connects to a capillary acting as a flow limiter as well as dilution air controlled by a mass flow controller that can be adjusted to a defined concentration for sensor calibration at ambient conditions (p, T, RH).

In order to capture the dynamic behavior of volcanic gas plumes, the UAV-based point measurements are supplemented by a lightweight spectrometer based on a mobile DOAS system.[3] This combination is intended to enable spatially resolved measurements of gas concentrations and fluxes in rapidly changing plume geometries. In the long term, the installation of an autonomous drone docking and charging station at Mount Etna is planned, allowing repeated automated measurement flights and near real-time data acquisition.

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Controlled Synthesis and Design of Highly Multiplexed Upconverting Nanoparticles for Live-Cell Imaging

Hyung Jun Kim[1,2], Alevtina Studenikina[1,2], Harrison W. Toll[1,2], Irmuun Tommy Altankhuyag[1,2], Ivana Hsyung[1,2], Kaibo Ma[1,2], João Shida[1,2], Caroline Kim[1,3], Y. Erin Chen[1,3], and Chunte Sam Peng[1,2]

[1]Broad Institute of MIT and Harvard, Cambridge, USA

[2]Department of Chemistry, Massachusetts Institute of Technology, USA

[3]Department of Biology, Massachusetts Institute of Technology, USA

Optical microscopy provides high-resolution insight into cellular organization and dynamics; however, current fluorescence methods are limited in multiplexing capacity and durability. Simultaneous multicolor imaging using fluorescent dyes is generally restricted to 4 colors.[1] Dyes suffer from photobleaching, hindering unique signals.[2] A new generation of robust, multiplexed optical probes would transform our ability to capture the full molecular and spatial complexity of living systems. Upconverting Nanoparticles (UCNPs) exhibit a unique anti-Stokes shift, converting near-infrared excitation into tunable, sharp emissions in the visible region with indefinite photostability and minimal autofluorescence. By changing lanthanide composition, the relative emission intensities can be precisely tuned to create distinct spectral "colors".[3]

Creating a large library of uniform, but spectrally distinct UCNPs presents a significant synthetic challenge due to the interdependence between composition and morphology. UNCPs' optical properties are dependent on nanocrystal size and uniformity, but varying dopant compositions to create different colors alters the nucleation and growth kinetics.[4] Typical three-step syntheses (ligand exchange, salt addition/drying, and high-temperature growth) require multi-parameter optimization for each individual color.

First, I report a novel, facile method allowing a synthesisze UCNPs wiht high control over nanoparticle formation while maintaining uniformity. By precisely tuning the temperature and duration of the second „drying" step, I found that nucleation kinetics could be modulated. This finding transforms the previously passive drying step into a useful control parameter, enabling the facile synthesis of uniform nanoparticles with sizes tunable from 8 nm to 170 nm.

Second, leveraging this new synthetic control, I designed and synthesized a highly multiplexed library of 20 spectrally distinct UCNPs with an average detection accuracy of 97.8%. This work successfully overcomes the kinetic challenges posed by varied dopant compositions and provides both a fundamental advance in $NaYbF_4$ nanocrystal formation and a practical toolkit for enabling highly multiplexed imaging, paving the way for more complex systems-level analyses.

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Coupling voltametric experiments and kinetic Monte Carlo simulations – Insights into hybrid all-Fe redox flow batteries

Alena Neudert[1,2],Steffen Zappe [2], Fridolin Röder [2], Christina Roth[1,2]

[1]*University of Bayreuth, Electrochemical Process Engineering, Bayreuth, Germany*

[2]*University of Bayreuth, Bavarian Center for Battery Technology (BayBatt), Bayreuth, Germany*

The growing demand for renewable energy resources requires durable and inexpensive technologies for large-scale energy storage to balance the fluctuations in power supply.[1,2] In this context, redox flow batteries (RFB) are a promising solution for stationary energy storage due to their scalability, modularity, and long cycle life.[1-3] Compared to the vanadium RFB as the most common technology in the field, the hybrid all-iron RFB offers a more cost-effective, non-toxic and earth-abundant alternative. However, the reduction from iron (II) to iron (0) in the charging process leads to inhomogeneous plating on the electrode and simultaneous parasitic hydrogen evolution reaction (HER).[1] Therefore, the all-Fe RFB requires further improvement and understanding of the ongoing processes.We investigated how changes of temperature, iron concentration and pH value affect iron plating and the HER by combining experiments and simulations. The two reduction processes are not separable electrochemically but can be deconvoluted by implementing the experimental data into our kinetic Monte Carlo (kMC) model: After parametrization of the kMC model, the experimental cyclic voltammograms (CVs) are mimicked by a fitted simulation and the model gives insights on and also predicts how hydrogen evolution and the deposition of iron are affected by various combinations of parameters. The approach to couple experiment and simulation enables us to gain fundamental mechanistic insights on the processes taking place on the electrode surface. Suggestions for further improvements to the battery's efficiency include a raise in temperature and a rough surface of the electrode.

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Designing Polymeric Adsorbents for Sustainable PFAS Remediation

Ahmet Cetinkaya[1], Belkacem Tarek Benkhaled[1], Mona Semsarilar[1]

[1]*Institut Européen des Membranes—IEM UMR 5635, Univ Montpellier, CNRS, ENSCM, 34090 Montpellier*

Per- and polyfluoroalkyl substances (PFAS) are highly persistent environmental contaminants due to the exceptional thermal and chemical stability of the carbon–fluorine bond.[1,2] Their widespread occurrence in water sources poses significant risks to human health, including hepatotoxicity, endocrine disruption, and immune system impairment, as well as serious ecological impacts.[3] The hydrophobic and lipophilic nature of PFAS makes them difficult to remove using conventional water treatment technologies, highlighting the urgent need for selective, sustainable, and reusable remediation strategies.[4]

In this work, we report the development of polymeric adsorbent materials with potential for selectively removing PFAS with diverse functional groups and chain lengths, which are also reusable and potentially scalable for industrial applications. Representative systems include crosslinked hybrid-hydrogels which can be tailored to target different PFAS compounds. These materials are straightforward and cost-effective to produce, offering high adsorption efficiency and reusability, providing a solid foundation for the development of sustainable and practical water treatment solutions capable of mitigating PFAS contamination and ensuring access to safe water.

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[2] C. Gomri, B. T. Benkhaled, M. Cretin, M. Semsarilar, Macromol. Chem. Phys. 2024, 225, 2400012.

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Electrochemiluminescence based on the formation of exciplex/ excimer

Chang-Ki Moon[1,2], Yuka Yasuda[3], Yu Kusakabe[3], Anna Popczyk[1], Shohei Fukushima[3], Julian F. Butscher[1], Nachiket Pathak[1], Joel Schlecht[4], Kuraudo Ishihara[3], Oliver Dumele[4], Hironori Kaji[3], Malte C. Gather

[1]*Humboldt Centre for Nano- and Biophotonics, Department of Chemistry and Biochemistry, University of Cologne, Cologne, Germany*

[2]*Organic Semiconductor Centre, School of Physics and Astronomy, University of St Andrews, St Andrews, United Kingdom*

[3]*Institute for Chemical Research, Kyoto University, Uji, Kyoto, Japan*

[4]*Institute of Organic Chemistry, Department of Chemistry and Biochemistry, University of Cologne, Cologne, Germany*

Used extensively in sensing applications, the application of solution-state electrochemiluminescent (ECL) devices, often referred to “fluid light”, in lighting and displays has been constrained by their low luminance and short operational lifetime. Here, we introduce ECL mechanisms based on exciplex[1] and excimer formations[2], leading to a significant improvement in the luminance, efficiency, and operational longevity of ECL devices, and demonstrate its use in a calligraphic display. Electrochemically induced hyperfluorescence (ECiHF) is achieved by using “double-decker” arrangement assumed by the electron donor and acceptor segments of the molecule TpAT-tFFO to realize thermally activated delayed fluorescence from an electrogenerated charge-transfer excimer state (Figure 1b) and a subsequent energy transfer to the rubrene emitter TBRb.

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[2] C.-K. Moon, Y. Yasuda, Y. Kusakabe, A. Popczyk, S. Fukushima, J. F. Butscher, N. Pathak, J. Schlecht, K. Ishihara, O. Dumele, H. Kaji, Malte C. Gather, Nat. Commun, 2026, in press.

Enabling activity-based protein profiling (ABPP) for drugs that form disulfides: identification of off-targets for an ALS drug candidate

Durgalakshmi Sivasankar[1], Wensheng Yang[1], Brandon Miller[1], Roman Manetsch[1], Jeffrey N Agar[1]

[1]*Department of Chemistry and Chemical Biology, Northeastern University, Boston, USA*

The toxicity of drugs often results from interactions with proteins other than the intended target. Identification of off-targets interactions is therefore a critical step in evaluating potential safety issues for existing and developmental drugs. The stability of the bonds between covalent drugs and their targets presents opportunities and challenges for analytical techniques. Those challenges have been addressed by chemoproteomics techniques for drugs that form carbon-sulfur bonds.[1,2] These techniques, however, cleave disulfide bonds are therefore not applicable to covalent drugs that form sulfur-sulfur bonds. Here we develop a desthiobiotin iodoacetamide (DBIA)-based chemoproteomics methods for the off-target ID of covalent drugs that form disulfides. We apply these to an advanced preclinical candidate for ALS, cyclic thiosulfinate (CT). A total of 11,215 reactive cysteine residues were profiled from 3,952 protein groups without missing values in a data independent acquisition (DIA) LC-MS/MS experiment with biological replicates (n=3). Many notable off-target interactions were identified and extrapolated to toxicological effect. In one example, Cys X in target Y (target identity will be disclosed at time of meeting. Currently filing a provisional patent) exhibited significant drug occupancy (93%). Irreversible binding of CT to this site may disrupt the protein's conformation, stability, or lipid droplet association, leading to partial or complete loss of function, even though this cysteine is not a part of the catalytic active site. Such a modification would mimic the protective effects of genetic loss-of-function variants in humans, potentially reducing hepatic lipid accumulation, inflammation, and progression of nonalcoholic steatohepatitis (NASH) and related liver diseases.

[1] Y. Liu, M. Patricelli, B. Cravatt, PNAS. 1999, 96, 14694-14699.

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Direct Mechanocatalysis – A novel technique for sustainable Catalysis

Maximilian Wohlgemuth[1],Maike Mayer[1], Lars Borchardt[1]

[1]*Ruhr-University Bochum, Inorganic Chemistry, Bochum, Germany*

The concept of direct mechanocatalysis is a novel concept of catalysis neither utilizing light, thermal heating nor electric potential as in conventional catalysis, but simply mechanical energy. In this mechanochemical approach the use of milling materials made from metals such as Pd, Ni, or Cu are both, catalyst, and energy transmitter and thus the addition of catalyst powder or advanced ligand system becomes obsolete. However, its scalability has been limited due to the cost of catalytically active metals and the wear of milling tools. Due to this issue we developed an electroplating concept, where simple steel materials were electroplated with the needed active catalyst metal.[1]

We first showcase this concept for a type of reactions that is commonly in the hand of homogeneous catalysis – C-C-cross coupling reactions catalysed by Pd and Cu. We show how various, even sterically-demanding and deactivated reagents, can be converted quantitatively in as little as 60 minutes via Suzuki-, Sonogashira-, Heck-, or Glaser coupling. We further advance this concept to the selective oxidation of alcohols to aldehydes using gold-coated milling balls.[2] Finally we show how even hydrogenation reactions can be conducted via this approach using milling vessels that are internally coated with Pd, Ru, Ni.[3] By translating this technique to reactive extrusion we were able to bring direct mechanocatalysis to large scale applications.[4]

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[2] M. Wohlgemuth, S. Schmidt, M. Mayer, W. Pickhardt, S. Graetz, L. Borchardt, Angew. Chem. Int. Ed., 2024, 63, e202405342

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Anomeric Amide-Enabled Alkene-Arene and Alkene-Alkene Aminative Coupling

Colin Stein[1], Jasper L. Tyler[1], Julius Wiener[1], Florian Boser[1], Constantin G. Daniliuc[1], Prof. Dr. Frank Glorius[1]

[1]*University of Muenster, Institute of Organic Chemistry, Muenster, Germany*

The development of new C–N coupling reaction has been a focus of extensive research in the past decades.[1] Despite constituting a valuable retrosynthetic transformation, methods to directly form two C–N bonds at a nitrogen center - without relying on heavily prefunctionalized building blocks - remain underdeveloped.[2,3]

In this work we showcase a new method for the aminative coupling of olefins and arenes, or two distinct olefins, directly at nitrogen. We designed a novel anomeric amide reagent, that is able to perform catalyst-free and highly regioselective olefin chloroamination reactions under very mild conditions, thereby inserting a nitrenoid precursor into the target molecule. Subsequent deprotection liberates the active nitrenoid species, which can then undergo intermolecular reactions with a wide variety of nucleophiles, all in a one-pot process.

Due to the simplicity of both the method and its building blocks, high-thoughput experimentation (HTE) was employed to rapidly explore the chemical space. The broad applicability was demonstrated through the modification of pharmaceutically relevant and structurally complex compounds giving rise to high value aziridines and 1,2-chloroamines.

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Spin-State Photoswitching in a [5]Helicene-Based Hydrocarbon

Takuma Miyamura[1],Lukas Jacob[2], Philipp Thielert[3], Sabine Richert[3], Stefano Crespi[2], Oliver Dumele[1]

[1]University of Cologne, Institute of Organic Chemistry, Cologne, Germany

[2]Department of Chemistry, Uppsala University, Sweden

[3]University of Freiburg, Department of Chemistry, Freiburg, Germany

Precisely controlling the spin state of molecular entities in a reversible manner is one of the longest standing challenges and motivations for scientists. It is especially challenging for stable and purely organic molecules because they are usually locked in a closed-shell electronic configuration.[1,2]

This contribution focuses on the development of helical photochemical spin-state switches.[3,4] Initially, 1,14-(±)-dimethyl[5]helicene was used in designing a photochemical switch with (meta) stable spin states. By introducing dimethylanthryl substituents at the 4th and 11th positions, the [5]helicene core undergoes photochemical retroelectrocyclization to form a paramagnetic species. The back reaction to its initial form 1-C can be triggered thermally or by quantum tunnelling at cryogenic temperatures. At high temperatures, a unidirectional rotational motion has been confirmed, making this system a unique spin-state photoswitch with light-driven molecular motor properties.

[1] P. ravat, T. Šolomek, D. Häussinger, O. Blacque, M. Juríček J. Am. Chem. Soc. 2018, 140, 10839–10847.

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The HyDRA blind challenge on microhydration: past, present and future

Margarethe Bödecker[1], Martin A. Suhm[1]

[1]*Georg-August University, Institute of Physical Chemistry, Göttingen, Germany*

The field of gas phase spectroscopy benefits from a robust interplay between quantum chemistry and experimental techniques. However, the vast array of available quantum chemical methods, coupled with the inherent limitations of experimental approaches, can lead to fortuitous and biased matches, particularly when the experimental outcome is known in advance. To facilitate the advancement of systematically enhanced quantum chemical predictions in vibrational spectroscopy and solvation science, we have organized the HyDRA (Hydrate Donor Red Shift Anticipation) blind challenge during the 2021/22 academic year within the framework of the DFG research training group BENCh.[1]

In this challenge, ten cold 1:1 complexes of organic molecules with water were prepared in a vacuum and examined by infrared and Raman spectroscopy for the first time. The fundamental vibration of the hydrogen-bonded water molecule (OH stretching) in these complexes was measured and kept secret until ten interested theoretical research groups worldwide had made their predictions in spring 2022. The detection of a robust anharmonic resonance in some of these water complexes[2] rendered this competition not only interesting for scaled harmonic predictions, but also for more elaborate anharmonic treatments.

This contribution describes the blind challenge from an experimental perspective and presents a survey on the performance of the various theory submissions.[3] An outline of the aim and focus of the second round of the HyDRA blind challenge (2025/2026) will be given.

[1] T. L. Fischer, M. Bödecker, A. Zehnacker-Rentien, R. A. Mata, M. A. Suhm, Phys. Chem. Chem. Phys., 2022, 24, 11442.

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Fair4Chem Award

The NFDI4Chem FAIR4Chem Award honors researchers in chemistry who publish exemplary research datasets that rigorously implement the FAIR principles (findable, accessible, interoperable, and reusable) thereby advancing transparency and data reuse in chemical research. Each year, the award recognizes the "FAIRest" chemistry dataset with a cash prize of 500 euros, funded by the Fonds der Chemischen Industrie, and highlights the awardee in a dedicated presentation at the JCF Spring Symposium, encouraging the broader community to share high-quality open research data.

Supplement Data of Anolytes for All-Iron Redox-Flow Batteries

Marius M. Engler[1], Michael Stich[1], Christoph Baumer[1], Andreas Bund[1]

[1]*Technische Universität Ilmenau, Germany*

Iron-based redox-flow batteries (Fe-RFBs) have gained attention as a promising option for stationary energy storage due to their use of cost-effective and environmentally friendly materials. Their efficiency and long-term stability depend strongly on the electrochemical properties of electrodes and, in particular, the electrolyte composition.[1,2] In this study, the fundamental characteristics of different base electrolytes and additives were investigated.[2]

Electrolytes containing iron sulphate or iron chloride were examined regarding their deposition behavior at room temperature. Kinetic data indicates advantages for simple electrolytes consisting of iron salt and supporting electrolyte at elevated pH (>2.0). However, long-term stability is limited by the oxidation of Fe^{2+}. In addition, an excess of complexing agents or buffers can significantly inhibit iron deposition, indicating that further optimization of additives and concentration ratios is required.[2]

To ensure reproducibility and comparability, this work provides datasets from experiments on iron-based half-cell electrolytes, including cyclic voltammetry combined with an electrochemical quartz crystal microbalance. The datasets include information on experimental setups, operating conditions, material properties, and data processing workflows.

The aim is to improve data acquisition and processing while standardizing data preparation and publication according to the FAIR principles. Publishing these datasets enhances transparency, supports reproducibility, and promotes collaboration in battery research while contributing to sustainable energy storage.

[1] Belongia, Shawn; Wang, Xiang; Zhang, Xin. Progresses and perspectives of all-iron aqueous redox flow batteries. Advanced Functional Materials, 2024, 34 (5), 2302077.

[2] Engler, Marius, et al. Investigating the Iron Plating and Stripping of Anolytes for All-Iron Redox-Flow Batteries. J, 2024, 7(4), 571-583.

Award for excellent supervision

The JCF Best Supervisor Award, presented by the JungChemikerForum of the German Chemical Society, honors exceptional PhD supervisors in the chemical sciences who demonstrate outstanding dedication to mentoring early-career researchers. This award recognizes supervisors who not only achieve scientific excellence, but also foster an inclusive, supportive research environment that promotes personal development, mental well-being, and fair, open scientific practice. By highlighting exemplary supervision, the award aims to strengthen a sustainable mentoring culture in academia and to showcase role models who empower the next generation of chemists.

Laudatio for Prof. Dr. Lena Daumann

Awardee: Prof. Dr. Lena Daumann, Laudatio: Pia Heinrichs

Heinrich-Heine-Universität Düsseldorf, Germany



The quality of supervision during doctoral studies is a decisive factor for the scientific success, motivation, and personal well-being of doctoral candidates. The Young Chemists Forum (JCF) of the GDCh is actively committed to improving doctoral conditions in the long term. A central component of this is the Best Supervisor Award. This award recognizes supervisors who, through their exceptional commitment and modern leadership culture, serve as role models for the scientific system. The aim is to highlight excellent supervision and reinforce the principle that good supervision should be the rule, not the exception.

This year, the jury is honouring Prof. Dr. Lena Daumann for her outstanding and holistic approach to supervision. She impressed with a comprehensive package that goes far beyond technical mentoring.

Her crisis management and empathy are particularly noteworthy: during the relocation of her research group, she found individual solutions for all doctoral students to enable them to continue their doctoral studies smoothly at the old location. In addition, Prof. Daumann, backed by her qualification as a mental health trainer, proactively integrates the promotion of mental health and the compatibility of family and career into her leadership style.

Her supervision concept is also characterized by excellent structural conditions, including regular development meetings and the targeted promotion of soft skills for career paths within and outside the academy. With her clear commitment to diversity, inclusion, and the FAIR principles, Prof. Dr. Lena Daumann exemplifies the values of responsible, modern, and humane supervision in chemistry.

We are delighted to invite you to a series of inspiring workshops hosted by our distinguished industry partners as part of the Spring Symposium 2026. These sessions are designed to equip you with practical skills, forward-looking insights, and valuable perspectives that extend beyond the laboratory. From strengthening your ability to make impactful decisions to exploring emerging technological frontiers and fostering inclusive innovation, our program offers opportunities for both personal and professional growth. Join us to gain guidance, exchange ideas with experts, and prepare confidently for the next steps in your scientific journey.

Focus matters: Strategic decision making @ ALTANA

Date: 10th of March 2026, 14:00 – 16:00

Location: Meet at registration desk, then Department of Chemistry, Seminarroom Exp 2

Organizer: Kristina Keisers, Fabian Stahl, ALTANA AG

Language: English

Description: This workshop explores the strategic decisions to be faced when a specialty chemical company has developed new technologies: How can you define the most promising application for the new product considering limited resources? Students identify key evaluation criteria, analyze information on product and applications and develop a reasoned recommendation. The workshop concludes with checking how AI can help with such decisions and discussing some real-life examples of strategic decision taking from ALTANA.

Einstieg in Generative KI und KI-Agenten für Labor und Forschung

Date: 10th of March 2026, 14:00 – 15:30

Location: Meet at registration desk, then Department of Chemistry, Seminarroom Exp 1

Organizer: Dr. Lorin Steinhäuser, Bayer AG

Language: German

Description: Ist der Hype schon vorbei oder können moderne KI-Agenten euch bei Ideenentwicklung, Recherche und anderen Alltagsaufgaben wirklich unterstützen? Dieser Workshop bietet einen kompakten Überblick über aktuelle LLMs und zeigt - insbesondere für KI-Einsteiger*innen - praxisnahe Prompt-Techniken, die sich direkt im Arbeitsalltag nutzen lassen. Im interaktiven Teil wendet ihr die Ansätze auf eigene Themen an und nehmt konkrete Impulse für einen produktiven Einsatz von KI mit.

CAVE

Date: 10th of March 2026, 14:00 – 16:00

Location: Meet at registration desk, then Department of Chemistry, Room tbd

Organizer: Daniel Wickeroth

Language: English or German

Description: The CAVE (Cave Automatic Virtual Environment) is a room whose walls, floor, and ceiling are projection surfaces that support stereoscopic displays. With stereo glasses, people in the CAVE have the impression of being in a three-dimensional computer-generated environment. In the CAVE, spatial structures and relationships can be grasped and better understood. This makes use of the human ability to move through complex spatial structures, estimate distances and proportions, and assess changes over time. Scientific findings can thus be obtained more efficiently. This can be used in all scientific fields where spatial organizational principles apply, e.g., molecular structures in chemistry, docking of active substances in drug development, formation of planetary systems in astrophysics, flow processes in nature and technology, interactions in brain structures, or the reconstruction of buildings at excavation sites.
Participants will also have the opportunity to bring their own 3D data to explore in the CAVE.

Excursion to Chempark Leverkusen

Date: 10th of March 2026, 12:40 – 17:30

Location: Meet at registration desk, then Kaiser-Wilhelm-Allee 101-103, 51373 Leverkusen

Organizer: Viviane Bayer

Language: English

Description: This industry excursion offers participants a unique opportunity to gain insight into the operations of the chemical industry at CHEMPARK Leverkusen, one of the largest chemical parks in Europe. The site is managed by Currenta, which provides infrastructure and services for numerous chemical and pharmaceutical companies located at the park. The visit begins at the central visitor reception, followed by a short introduction at the digital plant model, where participants will receive an overview of the site and its industrial structures. A guided bus tour through the site then provides impressions of the extensive production and infrastructure areas of the CHEMPARK. The programme concludes with a visit to the Environmental Analytics department, where participants will learn how environmental monitoring and analysis are carried out in practice. Overall, the excursion offers a rare behind-the-scenes look at the organisation, infrastructure, and environmental management of a major European chemical industry site.

The Diversity Catalyst: Accelerating Innovation in Science by Evonik

Date: 10th of March 2026, 14:00 – 17:00

Location: Meet at registration desk, then Department of Chemistry, Room OC 413.

Organizer: Björn Theis, Regine Trippe, Evonik Industries AG

Language: English

Description: In an era shaped by rapid technological advancement and global collaboration, diversity has emerged as a critical driver of scientific innovation. This interactive workshop explores how diverse perspectives, experiences, and identities fuel creativity and enable breakthrough solutions in research and development. Participants will be introduced to insights on the evolving role of diversity in science, gain an understanding of how variety strengthen team work and problem-solving and reflect on the impact of unconscious bias in scientific environments. Through discussion and practical exercises, attendees will uncover strategies to activate diversity as a catalyst for innovation and to build more inclusive, forward-thinking scientific communities.

Rethinking careers in Chemistry: is founding for me?

Date: 10th of March 2026, 14:00 – 16:00

Location: Meet at registration desk, then Department of Chemistry, Seminarroom C.

Organizer: Shanika Yadav, Sarah Schulz

Language: English

Description: The interactive workshop invites participants to explore entrepreneurship or intrapreneurship as a potential career path beyond academia. In the workshop participants will: Reflect on their individual motivations and career goals; discuss concerns, assumptions, and common misconceptions about founding; gain insights into the skills, mindset, and pathways of entrepreneurship and intrapreneurship; connect with experts from the startup ecosystem and have open conversations about topics related to founding; learn about available startup services and support programs. The workshop offers space to reflect, exchange ideas, and define next steps toward an entrepreneurial career.

Meet a Scientist - How to Science Communication in e.g. schools

Date: 10th of March 2026, 14:00 – 16:00

Location: Meet at registration desk, then Department of Chemistry, Seminarroom B

Organizer: Pia Heinrichs

Language: German or English

Description: In times of widespread online disinformation and science denial, making science accessible to the public is more important than ever. As many people have little direct contact with scientific research, there is scope for misunderstandings, fears and persistent stereotypes to arise. Science communication plays a vital role in counteracting these issues by building trust, fostering understanding and making scientific knowledge relevant to everyday life. At the same time, engaging in science communication provides scientists with a welcome break from their usual academic work and helps them to develop the vital skill of translating complex research into clear, accessible language.

In schools, chemistry is often perceived as particularly abstract, theoretical and intimidating. Through the Meet a Scientist initiative, Pia Heinrichs and Sophie Gutenthaler-Tietze are visiting schools across North Rhine-Westphalia to challenge these perceptions. By using vivid visual material from our research and sharing personal career stories, we aim to break down barriers, highlight diverse career paths and demonstrate that science is practical, exciting and accessible to all.

This workshop will present our Meet a Scientist concept, share our experiences, and offer inspiration and practical guidance for taking your first steps in science communication.

Berufseinstieg in der Chemie von VAA

Date: 10th of March 2026, 14:00 – 15:30

Location: Meet at registration desk, then Department of Chemistry, Lecture Hall III

Organizer: Pauline Rust & Ida Tolksdorf (lawyers at VAA), Hans-Georg Weinig (GDCh)

Language: German

Description: Mit welchen Gehaltsvorstellungen gehe ich in den Bewerbungsprozess?
Mit welchen Fragen kann man im Vorstellungsgespräch rechnen?
Welche Unterschiede gibt es zwischen der Arbeit in der Großindustrie versus dem Berufsalltag in kleineren und mittleren Unternehmen?
Dies sind nur einige Fragestellungen, auf die im Workshop eingegangen wird.
Daneben wird auch der Ablauf eines Bewerbungsverfahrens erläutert und konkrete Tipps für die verschiedenen Stationen des Bewerbungsverfahrens gegeben. Selbstverständlich besteht die Möglichkeit, konkrete Fragen rund um den Berufseinstieg zu stellen.

Scientific Publishing with Impact

Date: 10th of March 2026, 14:30 – 16:00

Location: Meet at registration desk, then Department of Chemistry, Seminarroom A

Organizer: Dr. Ulrike Kauscher Pinto

Language: English

Description: The publishing process is an integral part of building a career as a researcher. Recently, scientific publishing has undergone many changes and is continuing to develop rapidly. While high publishing standards, scientific integrity and speedy publication remain top priorities, important new developments like the use of GenAI are now also garnering greater attention.

This session offers an insider's perspective on scientific publishing, with a focus on editorial workflows, peer review, and strategies for successful manuscript publication. Dr. Kauscher Pinto will explore the value of publishing research, the editor's role in shaping scientific communication, and the key stages of the peer review process. Attendees will gain practical guidance on crafting impactful titles, abstracts, and cover letters to boost the visibility and influence of their work. Designed for early-career researchers, this talk offers actionable insights into navigating the publishing landscape and effectively communicating research to a global audience. The session will end with an informal Q&A during which you can ask any question you have regarding the publishing process!

Brewery Tour

Date: 13th of March 2026, 16:00

Location: Meet at registration desk, then Kalker Hauptstraße 260, 51103 Köln

Language: English

Description: Experience Cologne's brewing heritage at BRAUWELT KÖLN. Enjoy exclusive behind-the-scenes tours, discover traditional Kölsch craftsmanship, and taste authentic local brews in a historic setting. A must-visit for beer lovers and curious explorers alike!

Note: Preregistration is required. A participation fee of 15€ for students (student ID required) and 22€ for adults applies for the brewery tour. A payment should be made via PayPal Pool until Tuesday, 12:00.

Chocolate Museum

Date: 13th of March 2026, 15:30

Location: Meet at registration desk, then Am Schokoladenmuseum 1a, 50678 Köln

Language: English

Description: Discover the sweet side of Cologne with a visit to the famous Chocolate Museum, located directly on the banks of the Rhine. This interactive museum takes you on a journey through the history of chocolate, from its origins in ancient cultures to modern production processes.

Note: Preregistration is required. A participation fee of 13€ for students (student ID required) and 16.50€ for adults applies for the chocolate museum. A payment should be made via PayPal Pool until Tuesday, 12:00.

Cologne Cathedral Tour

Date: 13th of March 2026, 15:30

Location: Meet at registration desk, then Kölner Dom, Domkloster 4, 50667 Köln

Language: English

Description: Experience Cologne from a unique perspective! Join us for a visit to the South Tower of Cologne Cathedral, one of Germany's most iconic landmarks and a UNESCO World Heritage Site. After climbing approximately 500 steps, you will be rewarded with a breathtaking panoramic view over the city, the Rhine River, and the surrounding area.

Note: Preregistration is required. A participation fee of 4€ for students (student ID required) and 8€ for adults applies for the Cologne cathedral tour. A payment should be made via PayPal Pool until Tuesday, 12:00.

City Tour

Date: 13th of March 2026, 15:30

Location: Meet at registration desk

Language: English

Description: How about exploring Cologne's historic heart? Join a city tour through the vibrant Altstadt past iconic landmarks. Wander narrow, cobbled alleyways and lively squares like the Alter Markt to witness Cologne's transformation from Roman foundation to the present—in a 1.5-hour guided walking tour.

Note: Preregistration is required. A participation fee of 10€ applies for the city tour. A payment should be made via PayPal Pool until Tuesday, 12:00.

German Sport & Olympia Museum

Date: 13th of March 2026, 15:30

Location: Meet at registration desk, then Im Zollhafen 1 50678 Köln

Language: English

Description: How about exploring Cologne's historic heart? Join a city tour through the vibrant Altstadt past iconic landmarks. Wander narrow, cobbled alleyways and lively squares like the Alter Markt to witness Cologne's transformation from Roman foundation to the present—in a 1.5-hour guided walking tour.

Note: Preregistration is required. A participation fee of 7.50€ for students (student ID required) and 10.50€ for adults applies for the german sport & olympia museum. Guided tours are available for groups of more than 25 persons for 4€ per person. A payment should be made via PayPal Pool until Tuesday, 12:00.

Aera

The term "**aera**" is derived from the Latin word for "era" in English and "æra" in Danish. Our mission is also derived from our name – we want to create a new (a)era in IP consultancy.

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Aaera's attorneys have played significant roles in the creation and protection of landmark portfolios especially within the life science, medtech and electronics industries.

ALTANA Group: Global leader in true specialty chemicals

ALTANA is a global leader in true specialty chemicals. The Group offers innovative solutions for coating manufacturers, paint and plastics processors, the printing and packaging industries, the cosmetics sector, and the electrical and electronics industry. The product range includes additives, specialty coatings and adhesives, effect pigments, sealants and compounds, impregnating resins and varnishes, and testing and measuring instruments. ALTANA's four divisions, BYK, ECKART, ELANTAS, and ACTEGA, all occupy a leading position in their target markets with respect to quality, product solution expertise, innovation, and service.

Headquartered in Wesel, Germany, the ALTANA Group has 66 production facilities and 69 service and research laboratories worldwide. Throughout the Group, more than 8,000 people work to ensure the worldwide success of ALTANA. In 2024, ALTANA achieved sales of more than 3 billion euros. About 7 percent of the total sales is invested in research and development each year. Its high earning power and high growth rate make ALTANA one of the world's most innovative, fastest growing, and most profitable chemical companies.

BASF – Chemistry for Sustainable Innovation

BASF is one of the world's leading chemical companies, headquartered in Ludwigshafen am Rhein, Germany, with 234 additional sites across 92 countries. The company manufactures a broad portfolio of products and develops innovative solutions that are applied in numerous industries, including the automotive, construction and agricultural sectors.

BASF's vision is to enable its customers to achieve greater sustainability through innovation, while simultaneously undergoing its own transformation. The company has set the objective of becoming climate-neutral by 2050 and is actively working to improve the efficiency and sustainability of its production processes, energy use and product portfolio.

The successful implementation of these ambitions relies on a highly qualified and motivated workforce. BASF therefore seeks individuals who are committed to scientific excellence and who value the transformative potential of innovation. An entry into research and development offers access to a wide range of professional development opportunities. In addition to pursuing a scientific expert track or a leadership career within research and development, career progression into other functional areas of the company is also possible.

BearingPoint

BearingPoint is an independent management and technology consultancy with European roots and a global reach. The company helps organisations achieve sustainanle and measureable success – from strategy to implementation to operations.

BearingPoint operates in three business areas: traditional consulting, IP-based business serbices and software solutions. Bearing Point combines deep industry knowledge with technological expertise, particularly in the areas of digital transformation, data & analytics, regulatory requirements and sustainability.

BearingPoint's clients include many of the world's leading companies and organisations in industry, financial services and the public sector. BearingPoint's global network comprises more than 10,000 employees in over 75 countries. BearingPoint stands for partnership-based collaboration, practical solutions and the commitment to creating long-term value together with its clients.

Bayer AG

At Bayer, generalists and specialists, visionaries and passionate people, thinkers and doers come together to feed the world, slow climate change, and create healthier, more sustainable lives for all. And we do that by sharing knowledge, learning from each other, growing as people and professionals, expanding horizons, and turning ideas into real possibilities. We're real people with energy, initiative, curiosity, and dedication who want to drive positive and enduring change.

We invite you to explore diverse career opportunities where your expertise in chemistry directly shapes the future of Life Sciences. Whether you're advancing innovative formulations, driving breakthroughs in molecular research, or developing safer and more sustainable chemical solutions for health and agriculture: your work sets us apart as an employer of choice. At Bayer, your scientific skills make a tangible impact and contribute to products and technologies that improve lives worldwide. Discover how your passion for chemistry can fuel meaningful progress in a dynamic, cutting-edge, and inclusive workplace.

We all want to know who we might work with when exploring career options. Curious about what it's like to succeed at Bayer? Meet our people. Visit our career booth today and learn how Bayer employees solve challenges, affect change, grow into roles, and develop through mentoring and a supportive feedback culture. By nurturing our talent, we enable satisfying authentic careers and create a great place to work.



Carbolution

You The Chemistry – We The Chemicals

Carbolution supplies chemicals for research and development, from milligrams to tonnes. Our range of chemical, pharmaceutical and biotech products comprises around 2,500 items, most of which are available immediately from our warehouse in St. Ingbert. We are also happy to procure chemicals that are not listed in our catalogue on request.

Carbolution was founded in 2010 at Saarland University. Our strength lies in finding the best source for every chemical and delivering it quickly. Orders for products in stock that are received before 12 noon are delivered the next morning. Guaranteed and free of charge for deliveries within Germany.

With KEMBO relab chemicals, Carbolution also offers sustainable 'recycled chemicals' that were actually intended for disposal – some in their original containers and at significantly reduced prices.

CEM

At CEM Corporation, we develop advanced instrumentation for peptide and chemical synthesis, enabling scientists to move from concept to validated product with speed, precision, and confidence. Our technologies are engineered to enhance reaction control, improve reproducibility, and streamline laboratory and pilot-scale workflows across research, pharmaceutical, materials, and academic environments.

CEM is widely recognised for pioneering microwave-assisted solid-phase peptide synthesis (SPPS). Platforms such as Liberty Blue and Liberty PRIME deliver accelerated cycle times, enhanced coupling efficiency, and improved purity through precise temperature control and optimised reagent delivery. By reducing aggregation and minimising side reactions, our systems enable reliable synthesis of both routine and complex peptide sequences, supporting discovery, process development, and translational research: www.mikrowellen-synthese.de

Beyond peptides, CEM microwave reactors advance a broad range of chemical synthesis applications, including organic reactions, medicinal chemistry, polymer research, and materials development. Controlled microwave energy improves reaction kinetics and reproducibility while shortening development timelines. Integrated automation, intelligent software, and secure data management ensure traceable, audit-ready documentation suitable for regulated environments.

Carl ROTH
Chemicals, Laboratory Supplies, Life Science Products

For over 145 years, we have been offering expert advice and high-quality products for laboratories, scientific institutions and manufacturing companies.

Carl ROTH has its headquarters in Karlsruhe. From here, we supply our five branches in Europe and customers in over 100 countries worldwide. With over 42,000 items and our overnight delivery service, we are setting new standards in supplying our business partners.

We often develop our pioneering ROTH products on the basis of research projects and collaborations and in constant dialogue with our customers, making us the preferred partner for research, analysis and industry.

With our Green Solvents, we have created a genuine alternative to environmentally hazardous and harmful reagents. Sustainability is also achieved through the use of renewable raw materials and environmentally friendly manufacturing and recovery processes, and the ROTH for Future Score seal allows us to transparently show our customers the sustainability level of our products.

To ensure that you always find exactly what you need, we offer advice tailored to your individual requirements, with solutions that precisely match your needs. You benefit from our personalised cooperation, which is based on reliability, experience, top service and foresight – and all at a price-performance ratio that is unbeatable.

Carl Roth GmbH + Co. KG
Schoemperlenstraße 3 - 5
76185 Karlsruhe, Germany
www.carlroth.de

ChemVengers

We know building a company is not easy, especially if you are working in the chemical space. The ChemVengers will make your progress faster, acting as catalysts for your innovation. We help you translate scientific excellence into scalable applications by combining technical expertise with entrepreneurial know-how. Our thriving network includes experts covering all stages of the chemical value chain and is deeply embedded in the chemical startup ecosystem in Germany.

The ChemVengers are a Germany-wide alliance currently consisting of the following partners: Center for the Transformation of Chemistry (CTC), chemstars, Forum Rathenau e.V., greenCHEM, Hochschule Fresenius, koala Startup Network, Start4Chem, Startup Labor Schwedt, TUM Venture Labs ChemSPACE.

Join us at our booth to get to know more about the diverse programmes and challenges we are offering in regional parts as well as all over Germany. You can still apply for our current idea competition called the **"From Lab to Market Challenge"** until March 30th. Just scan the QR code or visit the following website: www.chemstars.de/fltmc



Currenta

The Currenta Group is an association of highly specialised companies under the umbrella of Chempark manager and operator Currenta, with subsidiaries Chemion, Tectrion, NetCUR and Ausbildungsinitiative Rheinland.

As a group, we have more than 100 years of experience in the chemical industry. Originating from the Bayer Group, we have developed from an internal service provider into a competitive group of specialists.

Currenta manages and operates one of the largest chemical sites in Europe – Chempark with its locations in Leverkusen, Dormagen and Krefeld-Uerdingen. As a modern service company, we create optimal research and production conditions for our customers based here. Our range of services includes, for example, on-site material and energy supply, a wide range of analytical services, modern environmental management, comprehensive infrastructure services and reliable safety concepts.

German Bunsen Society for Physical Chemistry young Physical Chemists

Physical chemistry uses interdisciplinary methods to fundamentally understand materials and chemical processes. With applications ranging from atmospheric chemistry to fuel cells, physical chemists are in high demand across research and industry. To support this broad and vibrant field, scientific societies like the German Bunsen Society for Physical Chemistry (DBG) play an essential role. The DBG connects scientists to share knowledge and foster collaborations. A key focus is nurturing early-career researchers through scholarships, awards, and the young Physical Chemists, who organize networking and career-planning events to connect young talent with industry and academia.



Free membership for Bachelor, Master & PhD students!

Deutsche Bunsen-Gesellschaft für physikalische Chemie

www.bunsen.de | www.bunsentagung.de | www.bunsen.de/ypc

young PHYSICAL CHEMISTS

@ypc_bunsen young Physical Chemists

Enamine

Founded in 1991, Enamine has grown into a leading global provider of screening compounds, building blocks, and fragment libraries, supporting early drug discovery efforts worldwide. With decades of experience and a strong foundation in medicinal and synthetic chemistry, as well as HTS and preclinical biology we collaborate with pharmaceutical and biotech companies, academic institutions, and research centers to accelerate innovation in the life sciences.

In 2023, we expanded our presence to Frankfurt am Main, establishing a dynamic site focused on FTE chemistry support, custom synthesis and medicinal chemistry services – including Hit-to-Lead optimization, SAR studies, and route scouting.

Our international team in Frankfurt consists of around 30 highly skilled scientists specialized in the design and synthesis of complex small molecules, focused compound libraries, peptidomimetics, and macrocycles, combining conventional wet chemistry with innovative parallel synthesis techniques. At Enamine, we value scientific excellence, collaboration, and creativity. Enamine offers a unique opportunity to work at the forefront of drug discovery in a fast-paced, collaborative, and supportive environment.

Evonik Industries AG

Evonik is a leading global specialty chemicals company headquartered in Essen, Germany, with activities in more than 100 countries. In 2024, the company generated €15.2 billion in sales and €2.1 billion in adjusted EBITDA. With around 32,000 employees worldwide, Evonik is committed to creating real competitive advantages for customers through innovative materials, advanced technologies, and tailor-made solutions that improve people's lives.

As a driver of industrial and societal transformation, Evonik pushes the boundaries of chemistry and collaborates closely with the scientific community and industry partners. Together, we develop forward-looking solutions such as lipids for next-generation medicines, biosurfactants for sustainable detergents, additives that enable plastic circularity, and high-performance membranes supporting the energy transition.

At Evonik, scientific progress is deeply connected to personal growth and meaningful impact. We encourage unlimited potential, embracing curiosity and the desire to explore complex challenges. In a supportive environment where you are valued and heard, you will collaborate with experts across disciplines and countries to advance innovation in materials science, chemical engineering, biotechnology, and sustainability. Join Evonik and be part of something special, become a builder of the future and think beyond chemistry.

FCI (Fonds der Chemischen Industrie)

The **Fonds der Chemischen Industrie** is the funding organisation of the **Verbands der Chemischen Industrie e.V**. Since 1950, it has been supporting education and science in the field of chemistry in Germany with funds from the chemical and pharmaceutical industry. Its aim is to strengthen research, promote young scientists and ensure the long-term quality of academic education.

Its activities focus on **supporting young scientists:** the fund awards scholarships to doctoral students and prospective university lecturers, promotes research projects by young scientists and provides funding for the further development of new teaching content in chemistry studies and chemistry-related disciplines.

Another key focus is the promotion of chemistry teaching in schools. The fund **supports experimental and modern science teaching** – from primary school to secondary school. This includes the free provision of teaching materials on current topics, financial assistance for equipping specialist classrooms, and the promotion of projects designed to spark young people's interest in chemistry.

Furthermore, the fund awards prizes and honours, e.g. to outstanding scientists, and supports school competitions. It also supports scientific conferences that serve to exchange new research results and integrate young researchers into the scientific community.

Overall, the Chemical Industry Fund thus contributes to sustainably strengthening education and research in chemistry, promoting young talent, and continuously improving the quality of science education in Germany.

Further information can be found on the fund's official website: www.vci.de/fonds/startseite.jsp

FACCTs

FACCTs is a spin-off of the Max-Planck-Society founded in 2016. Our mission is to bring academic innovation to industry, providing fast and accurate simulation tools for chemical, materials and pharmaceutical R&D.

Originally founded with the goal to license ORCA, FACCTs soon became a valuable link between academia and industry. Since then, we have extended cutting-edge academic methods in order to tailor them to our customers requirements.

Together with our partners, we develop new algorithms and methods to push accuracy and efficiency to their limits and define the new state-of-the-art in quantum chemistry.

With a user base of about 100000 users and more than 70 industry partners it is used by scientists in their daily work to solve all kinds of problems using actual physics-based models built around solving the Schrödinger equation.

Grünenthal GmbH

Grünenthal is a global leader in pain management and related diseases. As a science-based, fully integrated pharmaceutical company, we have a long track record of bringing innovative treatments and state-of-the-art technologies to patients worldwide. Our purpose is to change lives for the better – and innovation is our passion. We focus all our activities and efforts on working towards our vision of a World Free of Pain.

Grünenthal is headquartered in Aachen, Germany, and has affiliates in 28 countries across Europe, Latin America, and the U.S. Our products are available in approx. 100 countries. In 2024, Grünenthal employed around 4,300 people and achieved revenues of €1.8 billion.

More information: www.grunenthal.com

Forschungszentrum Jülich

Conducting research for a changing society: This is what drives us at Forschungszentrum Jülich. As a member of the Helmholtz Association, we aim to tackle the grand challenges of our times. How can we utilize the potential of artificial intelligence for society and science? How can we decode the human brain? How can we make a success of the energy transition and mitigate the effects of climate change? And how can we facilitate the transition to a sustainable economy in regions affected by structural change? Come and work with us at our scientific institutes, administration, or in research management alongside around 7,700 colleagues from almost 110 countries at one of Europe's biggest research centres and help make a contribution to solving societal challenges. Help us to shape change!

As a university student, you have the opportunity to gain practical experience alongside your studies, expand your knowledge and make a meaningful contribution to socially relevant issues through your work:

- An internship or practical semester allows you to gain initial insights into the work at Forschungszentrum Jülich, apply your previous knowledge and gain valuable experience.
- As a student assistant, you are directly integrated into the daily research and work routine - you support our colleagues in their daily tasks and thus make an important contribution through your work.
- For your bachelor's or master's dissertation, we offer you the opportunity to work independently on current topics and research questions. We ensure comprehensive professional supervision to support you in the best possible way.

For more information on career opportunities, visit www.fz-juelich.de/careers.

Learn more about the values, mission and vision of the Research Centre in our mission statement: https://go.fzj.de/leitbild

IMCD

Die IMCD-Gruppe ist ein weltweit führender Distributionspartner, Formulierer und Lösungsanbieter von Spezialchemikalien und Ingredienzien. Mit einem globalen Netzwerk aus Branchenexperten bieten wir unseren Lieferanten und Kunden in den Regionen EMEA, Amerika und im asiatisch pazifischen Raum marktorientierte Lösungen sowie ein umfassendes Produktportfolio und innovative Formulierungen für die Bereiche Home Care and I&I, Beauty & Personal Care, Food & Nutrition und Pharmaceuticals bis hin zu Lubricants & Energy, Coatings & Construction, Advanced Materials und Industrial Solutions. Im Jahr 2025 erzielte die IMCD-Gruppe mit Hauptsitz in Rotterdam mit über 5.200 Mitarbeiterinnen und Mitarbeitern in über 60 Ländern auf sechs Kontinenten einen Umsatz von 4,8 Milliarden Euro.
1996 eröffnete IMCD Deutschland als eine der ersten Tochtergesellschaften seinen Hauptsitz in Köln. Dieser wird heutzutage durch einen strategischen Standort in Hamburg, sowie Labore für die Bereiche Pharmaceuticals, Food & Nutrition, Coatings & Construction und Home Care and I&I in Köln ergänzt. Deutschlandweit arbeiten aktuell rund 270 Experten an immer neuen Lösungen für den Erfolg unserer Geschäftspartner.

Merck

Merck is a leading science and technology company, with a rich history dating back to 1668. The company is committed to sustainability and innovation, investing significantly in research and development. We are dedicated to improving lives and enhancing the quality of life through our diverse portfolio of products and solutions. The Sigma-Aldrich brand, a part of Merck, plays a crucial role in supporting chemists by providing high-quality reagents, innovative tools, and comprehensive solutions that empower researchers to make significant advancements in their work. Through this brand, we continue to foster scientific progress and collaboration within the global research community.

NFDI4CHEM

NFDI4Chem (the chemistry-consortium of the National Research Data Infrastructure) stands for a simple idea: good chemistry needs good data – FAIR, i.e. findable, accessible, interoperable and reusable. To this end, the consortium is setting up a digital infrastructure specifically for chemistry and developing standards that will enable spectra, reaction data and simulations to be described in a uniform manner and made machine-readable. For you as a chemist, this means that You can publish your research data just as easily as your article – with DOIs, clear metadata and without having to study IT.

NFDI4Chem supports you with repositories, electronic lab books, guidelines and training courses so that research data management is not an additional burden, but saves you time, makes your results more visible and puts your scientific career on a professional footing right from the start.

Reloc RTG 2550

Biological systems are astonishingly adaptable. Cells employ dynamic protein (re)localization as central mechanism to expand proteome complexity and to allow cellular adaptation to a multitude of intra- and extracellular signals. The mechanisms driving and controlling (re)localization events, and their functional and physiological consequences are only poorly understood.

In 2020, our research training group funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) began to explore this layer of regulation and proteome complexity-expansion. Based in Cologne, this project brings together PhD candidates from both University of Cologne and Max Planck Institute for the Biology of Ageing with their backgrounds ranging from biology over biochemistry to organic chemistry.

The RTG does not only provide a financial and organizational framework to perform research but also heavily invests in the personal development of each PhD student. In several workshops, our PhD students improve scientific competences and soft skills and in our Reloc Seminar Series we invite experts from all over the world to connect with us and share their insights and experiences. Therefore, we are happy to support the Spring Symposium 2026 by inviting Michal Hocek for a Keynote Lecture.

TIDE (Template-Designed Organoelectronics) RTG 2591

TIDE is a DFG-funded Research Training Group providing a comprehensive doctoral education program in the field of Organic Electronics. Our team of more than 13 expert researchers strengthens TIDE in terms of breadth, complexity and interdisciplinarity coming from different disciplines like Physical, Organic, and Theoretical Chemistry, as well as Physics and Materials Science, and is located at at the two universities University of Cologne, and University Bonn.

The goal of our research is to understand how one-dimensional (1D) templates influence the structural ordering of molecular building blocks and, consequently, charge transport in π-conjugated materials.

Complementing research, TIDE offers a structured training program with joint lecture series in Chemistry, Physics, and Materials Science, a certified Bench-to-Business (B2B) course bridging fundamental and applied research, dedicated key skills training, and a mandatory three-month international research stay.

According to our philosophy that scientific success necessitates encompassing exchange, we are pleased to invite Luisa de Cola as a Keynote Speaker for the Spring Symposium 2026.

Thieme – Empowering Chemists.

We provide authoritative and expertly curated information in organic, sustainable, and medicinal chemistry — supporting professional chemists and advanced students.

Our journal portfolio features leading peer-reviewed publications such as SYNLETT, SYNTHESIS, and SynOpen, complemented by our newest additions, Sustainability & Circularity NOW and Therapeutics NOW. Beyond journals, we offer a suite of trusted reference solutions, including the synthetic methodology resource Science of Synthesis, the comprehensive guide Pharmaceutical Substances, and the renowned chemical encyclopaedia ROEMPP.

At Thieme Chemistry, close collaboration across product development, editorial, marketing, and sales drives the creation of innovative digital products that empower chemists worldwide.

tesa SE

As a multinational company, tesa develops innovative adhesive tapes and self-adhesive product solutions for various industries, commercial customers, and end consumers. Already more than 7,000 tesa adhesive solutions help improve the work, products or lives of our customers. Today, the focus is on sustainability and energy-saving processes. tesa invests in the development of environmentally friendly products and solvent-free manufacture processes as well as in the use of renewable energy sources at its locations.

tesa is active in 100 countries and operates plants in Germany, Italy, China, USA, and in Vietnam. Around three quarters of the tesa Group's sales (2023: EUR 1.7 billion euro) are generated by applications for industries. Together with its international clients, tesa develops innovations that are customized at product and process level. Already more than 130 tesa tapes may be installed in an electric car and over 70 in a smartphone. In the printing and construction industries, too, tesa is constantly penetrating new segments and countries with its special adhesive tapes. The company generates almost one quarter of its sales with products for end consumers and professional craftsmen. 300 applications, such as the legendary tesafilm®, make life easier or, when it comes to insect protection, even make it a bit more pleasant. tesa counts among the world's leading manufacturers of adhesive solutions. Since 2001, tesa SE is an independent 100% affiliate of Beiersdorf AG (i.e., NIVEA, Eucerin, la prairie) with approx. 5,200 employees.

VAA

Der VAA ist die Interessenvertretung der Fach- und Führungskräfte in der chemisch-pharmazeutischen Industrie und den angrenzenden Branchen – seit über 100 Jahren. Wir stärken unsere Mitglieder für ein erfolgreiches Berufsleben und darüber hinaus. Das ist Sinn und Zweck unseres Handelns – bei der Vertretung der Mitgliederinteressen gegenüber Arbeitgebern, Politik und Gesellschaft ebenso wie bei der individuellen Unterstützung in Ihrem Berufsleben. Wir arbeiten mit Leidenschaft und wir halten zusammen. Unsere Mitglieder sind vor Ort in Betrieben, an den Standorten und unternehmensübergreifend organisiert: 30.000 Fach- und Führungskräfte in 170 Werksgruppen und acht Landesgruppen. Wir sind offen für die Vielfalt von Berufsbildern und Karrierewegen in unserem Branchenumfeld. Wir vertreten mit Leidenschaft die Interessen unserer Mitglieder als versierte Gewerkschaft, persönlicher Unterstützer und aktiver Multiplikator. Wir pflegen Netzwerke und leben Community. Wir kennen, teilen und heben den Mehrwert des Miteinanders. Wir sind durch Professionalität, Wissen und organisatorische Stärke ein verlässlicher Partner – für unsere Mitglieder und unsere Partner.

Posters in Session 1

P1 Buse Özsan: The Effect of Organic Sensitizers Containing 1,10-Phenanthroline Anchor Group and Lanthanide-Doped Ag-TiO_2 Semiconductor on The Performance of Dye-Sensitized Solar Cells

P2 Kaan Şendal: Photocatalytic Degradation of Binary Dyestuff Mixtures Using Green-Synthesized Zinc Oxide Nanoparticles

P3 Sinan Yurdakul: Synthesis of Bridge-Functionalized Norbornene Monomer and Its Polymerization via ROMP

P4 Kadir Turhan: Synthesis and Investigation of New Ninhydrin Derivatives for The Development of Latent Fingerprints

P5 Janina Carolin Höner: The novel LMU-2 zeolite structure and its transition to chabazite

P6 Marcela de Barros: Empowering the Next Generation of Chemists: NSYCC Initiatives for Career Development and Community Building

P7 Karla Heckhäuser: Multi-Thermoresponsive LCST-UCST Diblock Copolymers in Water

P8 Elmas Kırtay: Encapsulated Phase Change Materials in Polypropylene Composites

P9 Aylin Pak Kaymaz: Starch–PAMAM Dendrimer Hybrid Gels for Controlled Urea Release and Sustainable Fertilization

P10 Nazli Kaya: Waste-to-Value: Development of Green and Innovative Materials from Renewable Resources for Boron Adsorption via Photoinduced Inverse Vulcanization

P11 Durgalakshmi Sivasankar: Enabling activity-based protein profiling (ABPP) for drugs that formdisulfides: identification of off-targets for an ALS drug candidate

P12 Anant Onkar Bhasin: Plasmon decay pathways in magic sized nanoclusters: Hot-carrier dynamics for photocatalyst design

P13 Hannah Lynn Harrison: Characterizing Defects in InP Quantum Dots through Structural and Optical Characterization of InP Magic-sized Clusters

P14 Lilly Meynberg: Predicting the Stability of Base-mediated C–H Carboxylation Adducts Using Data Science Tools

P15 Hatice Kübra Erdogan: Investigation of Thermodynamic Properties of White Benzoin by Inverse Gas Chromatography Method

P16 Sophie Wagner : Diels-Alder-Based Thermoreversible Silicone Networks

Poster Presentations

P17 Ömer Tuğcu: Synthesis and Characterization of Novel Thienyl-Methylene Substituted 1,3-Thiazolidinone Derivatives

P18 Margarethe Bödecker : The HyDRA blind challenge on microhydration: past, present and future

P19 Kathrin Kolling: Synthesis and characterisation of amphiphilic, metal-containing block copolymers via anionic polymerization

P20 Ceren Can Karanlık: Novel Furan Ring-Based Rod-Shaped Molecules: Synthesis, Characterization and Investigation of Mesomorphic Properties

P21 Tim Schramm: A 100,000-Fold Increase in C-H Bond Acidity Gives Palladium a Key Advantage in C(sp3)-H Activation Compared to Nickel

P22 Irene Böck: Young Chemists Network (JCF) Ulm

P23 Elisabeth Sennert : OH NO! – The microsolvation of TEMPO derivatives in the gas phase

P24 Pascal Dippner: Mechanochemical room-temperature synthesis of C2N-type materials from HATCN and its precursors

P25 Alina Kasberg: Temperature-Triggered Depolymerization of Dilution-Resistant Supramolecular Polymer Bottlebrushes

P26 Johanna Koll: Control of self-assembly of supramolecular polymer bottle brushes based on benzene tripeptides via microfluidics

P27 Thokozire E. Sweetland: Functionalized Initiators for Anionic Polymerization: Investigating the Relationship between Structure and Reactivity in Ethers

P28 Nils Wegerich: Reactivity of Platina(II)pnictinidenes with Maleic Anhydride

P29 Maike Mayer: Gas meets Solid – Gas-mechanochemistry for catalytic reactions

P30 Sören Steup: Alkylthio aurone fluorophores: a structure–property relationship of emission in solution and in the solid state

P31 Karolina Trojanowska: Fabrication and characterization of a hydroxyapatite-containing biodegradable polymer composite

P32 Elif Çeltek: Solid State Synthesis of Quantum Dots and Investigation of Dye Adsorption Properties for Waste Treatment

Poster Presentations

P33 Milena Waldhoff: Propagation and Depropagation Kinetics of Tetrahydrofurfuryl Methacrylate Investigated by PLP-SEC

P34 Tamilarasu Ganeshamurthy: Simultaneous Pressure-Temperature Dependent Luminescence Response of the Eu3+-Activated BaGeO3

P35 Daniel Kösters: Covalent polymeric composite materials for gas separation membranes

P36 Samuel Wendler: Radical Depolymerization Under Aspects of Sustainability

P37 Daniil Knyazev: Dimerization Reactions of of Aryl-Substituted Bicyclobutanes (BCBs) under Acid-promoted Conditions

P38 AK Siewert: Sophie Dequiedt, Frederick Giebelhausen, Hanna Graf, Lewis Hess, Amelie Rein: Redox Reactivity of Triarylboranes

P39 Alina Bauer: Cooperative Asymmetric Catalysis Under Confinement

P40 Alexandra Tietze: Working Under Pressure: Empirical Findings on the Challenges Facing PhD Students in Chemistry

P41 Snežana Tošić: Effect of Natural Zeolite (Clinoptilolite) on Heavy Metal Content in Lemon Balm (Melissa officinalis L.)

P42 Aleksandra Pavlović: Effect of thermal processing on polyphenol content, flavonoids, and antioxidant activity of Rosa dumalis Bech. fruits

P43 Inga Lene Schneider: London Dispersion Stabilized meta-Bisazobenzenes – Combining New Concepts for MOST Applications

P44 Sophie Richter: Characterization of the Initial Lithiation Step in FeS2 All-Solid-State Lithium-Sulfur Batteries

P45 Benedikt Bädorf: Efficient Prediction of Singlet-Triplet Gaps at DFT Accuracy Using the g-xTB Method

P46 Marla Brandstäter: Tuning of Arsenic Corrole Complexes by Axial Coordination: From Photophysics to Photosensitization

P47 Alena Neudert: JCF Team Mentale Gesundheit

P48 Anna-Lisa Poser: Shape Memory Polyurethane Foams: Innovative Solutions for Safer and Sustainable Applications

Poster Presentations

P49 Martin Behringer: Novel Azaborine-Based Inhibitors of Histone Deacetylases (HDACs)

P50 Marvin Friede: Advancing Dispersion Corrections in Computational Chemistry

P51 Alice Cappitti : Turning lignocellulosic biomass into sustainable polymer materials

P52 Steffi Krause Hinojosa: Mechanochemical Control of the Dehydration Degree of $CuSO4{\cdot}5H2O$ by Vessel Material

P53 Edvards Bensons: Selective Boost of Spin Diffusion Pathways under Site-Specific DN

P54 Malwine Lühder: Low dimensional perovskites in metal halide perovskite solar cells

P55 Tim Stamp: Decarboxylative Arylation yields novel -Amino Acids via Nickel Photoredox Catalysis

P56 Marie-Désirée Schlemper-Scheidt: Functional characterization of the C. elegans' mitochondrial 2-ketoacylCoA thiolase (kat-1) using comparative metabolomics

P57 Niklas Padberg: An economic-chemical view of the global distribution of raw materials, resources and reserves for the production of Sodium-Ion Batteries

P58 Niklas Rimkus: Computationally assisted engineering of urethanase activity

P59 Lars Georg: Polydentate, binucleating Ligands for Cu(I) dioxygen adduct formation

P60 Jonas Schnau: Young Chemists Network (JCF) Bayreuth

P61 Lorenz Crome: Is it possible to coordinate two metal centers via a bis(amino)acetylene ligand?

P62 Clara Schritt: A Diastereoselective Synthesis of small αα Calix[4]pyrrole Building Blocks

P63 Janos Wasternack: A Scalable and Resource-Saving Synthesis of Dipyrromethanes and Tetrapyrroles - Minimal Polymer Formation and Facile Purification

P64 Clarence Yong: Colourful Pertechnetates: From Simple Salts to Subtle Bonds

Poster Presentations

P65 Veselina Adımcılar: Sustainable Design-Oriented Biopolymeric Platforms for Visual pH Sensing

P66 Pia Heinrichs: Laudatio Best Supervisor Award – Award for best supervision

P67 Sabrina Even: Paleobiotechnology: Using ancient DNA for natural product discovery

P68 Takuma Miyamura: Spin-State Photoswitching in a [5]Helicene-Based Hydrocarbon

P69 Julian Burkhart: Recovery of Germanium from Germanium Dioxide Using Hydrogen or Natural Gas in Chemical Vapour Transport Processes

P70 Philipp Holz: Targeting fibrin with EPep: A peptide probe for stroke research

P71 Soyoung Boo: Highly Efficient Thermally Activated Delayed Fluorescence (TADF) OLED under Strong Exciton-Photon Coupling Showing Narrowband and Tuneable Emission

P72 Jan van Stiphoudt: Illuminating Artemisinin: A Photochemical Approach to Unlock Its Pharmacological Potential Beyond Malaria

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P1

The Effect of Organic Sensitizers Containing 1,10-Phenanthroline Anchor Group and Lanthanide-Doped Ag-TiO_2 Semiconductor on The Performance of Dye-Sensitized Solar Cells

Buse Ozsan,[1] Ibrahim Erden[1]

[1] *Yıldız Technical University, Faculty of Arts and Sciences, Department of Chemistry, Istanbul, Türkiye*

Dye-sensitized solar cells (DSSCs), recognized as third-generation photovoltaic technologies, have attracted significant attention as promising alternatives to silicon-based solar cells due to their low production costs, simple fabrication processes, and tunable optical properties. The operating principle of DSSCs was first introduced by O'Regan and Grätzel, who demonstrated the use of a photosensitizing dye coupled with a mesoporous TiO_2 semiconductor.[1] Efficient intramolecular charge transfer (ICT) through a conjugated π-bridge is essential for achieving high power conversion efficiency (PCE). In this study, imidazole bridge units were incorporated into sensitizer designs to promote directional electron transfer, while 1,10-phenanthroline was employed as the anchoring group to ensure effective binding to the TiO_2 surface.[2,3] The L1 molecule was synthesized by reacting N-(4-formylphenyl)carbazole-formed from 4-chlorobenzaldehyde and carbazole-with 5,6-diamino-1,10-phenanthroline under anhydrous conditions, proceeding via imidazole ring formation.[4] Structural characterization was elucidated using FTIR, ^{1}H-NMR, Q-TOF MS and UV-Vis analysis. Additionally, to further enhance electron transport within the semiconductor, Ag-TiO_2 films were doped with Gd^{3+} and Tb^{3+} ions at various ratios. Photovoltaic performance of the fabricated devices was evaluated under a solar simulator using current–voltage (I-V) measurements. Overall, both the sensitizer design and the semiconductor modification enabled the development of DSSC devices with enhanced cell performance. In particular, the incorporation of lanthanide ions into the semiconductor material resulted in a significant improvement in power conversion efficiency.

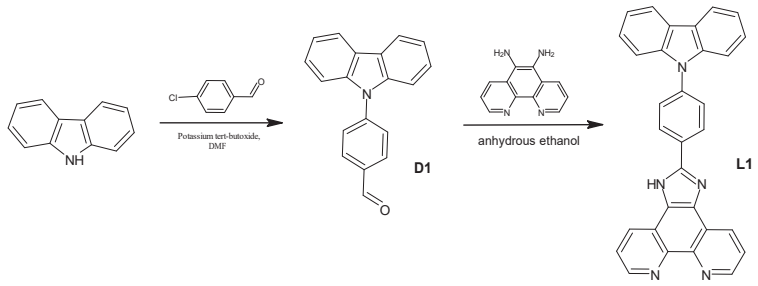

Figure 1: Synthesis scheme of sensitizer

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Photocatalytic Degradation of Binary Dyestuff Mixtures Using Green-Synthesized Zinc Oxide Nanoparticles

Kaan Şendal,[1] Mahmure Üstün Özgür,[1] Öznur Dülger Kutlu[1]

[1] *Yildiz Technical University, Faculty of Arts and Sciences, Department of Chemistry, Istanbul, Turkey*

Synthetic dyestuffs are widely used in many sectors, particularly the textile industry. They are persistent pollutants that accumulate in aquatic ecosystems, causing toxic, mutagenic, and carcinogenic effects.[1] In cases where conventional treatment methods are insufficient or produce secondary waste, photocatalytic degradation processes using metal oxide nanoparticles such as zinc oxide nanoparticles (ZnONPs) stand out as an effective advanced oxidation process for completely mineralizing pollutants.[2] However, industrial wastewater usually contains not a single pollutant but a mixture of dyestuffs with different chemical structures. In such complex matrices, classical absorbance measurements are insufficient due to the overlapping spectral bands of the dyestuffs, making it difficult to simultaneously analyze and monitor the degradation of mixed pollutants. In this context, the derivative spectrophotometric method, which is one of the advanced spectrophotometric methods for the analysis of mixtures, stands out.[3]

In this study, ZnONPs were synthesized via an environmentally friendly green synthesis method using plant extracts. The synthesized nanoparticles were characterized by UV–Vis, FTIR, FESEM-EDS, and XRD analyses. The main objective of the study was to evaluate the dyestuff removal performance of green synthesized ZnONPs in the photocatalytic degradation of binary mixtures of Methylene Blue, Basic Yellow 28 and Basic Red 18 dyestuffs simulating real wastewater conditions. The spectral overlap problem encountered in the mixtures was overcome by applying the first derivative UV–Vis spectrophotometry method, and the degradation of each dyestuff was monitored simultaneously. The obtained results demonstrate that the green synthesis-derived ZnONPs exhibit high photocatalytic activity even in complex systems containing multiple pollutants, making them a sustainable nanocatalyst candidate for water treatment.

Keywords: green synthesis, zinc oxide nanoparticles, binary dyestuff mixture, derivative spectrophotometry

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P3

Synthesis of Bridge-Functionalized Norbornene Monomer and Its Polymerization via ROMP

Sinan Yurdakul[1], Prof. Dr. Tarık Eren[1]

[1] Yıldız Technical University, Faculty of Arts and Sciences, Department of Chemistry, Istanbul, Türkiye

The development of functional norbornene monomers offers unique opportunities to design polymers with tunable chemical and physical properties using ring-opening metathesis polymerization (ROMP).[1] In this study, we report the synthesis of a norbornene derivative bearing a substituent introduced through the bicyclic bridge position, enabling the introduction of hydrophobic aromatic-alkyl segments directly into the polymer backbone. (Figure 1) The monomer was prepared through a nucleophilic substitution strategy, followed by structural confirmation using FTIR, $^{1}H/^{13}C$ NMR spectroscopy.[3] Subsequent polymerization was carried out using a ruthenium-based ROMP catalyst (Grubbs-type), and the reaction parameters—including solvent effects, monomer concentration, and catalyst loading—were systematically evaluated to obtain high-molecular-weight polymers with controlled dispersity.[1]

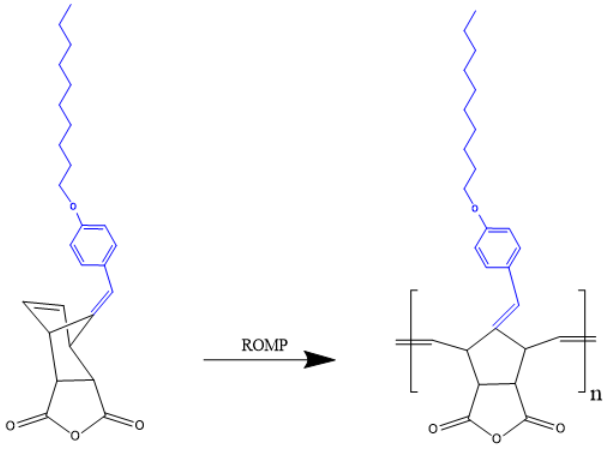

Figure 1: Schematic representation of the synthesized bridge-functionalized norbornene monomer and its polymerization via ring-opening metathesis polymerization (ROMP).

The resulting bridge-functionalized ROMP polymers exhibited distinct thermal behavior, hydrophobicity, and tunable chain packing characteristics.[2,4] The incorporation of bridge-functionalized side groups also imparted potential for intermolecular interactions, suggesting applicability in coatings, compatibilizers, or amphiphilic polymer systems.[4]

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P4

Synthesis and Investigation of New Ninhydrin Derivatives for The Development of Latent Fingerprints

Mehmet ULUER, [1] Kadir TURHAN, [1]

[1] *Yıldız Technical University, Department of Chemistry, İstanbul, Turkey*

Fingerprints are among the most important biometric data used in forensic and administrative procedures. Latent fingerprints (LFPs) are transferred to the touched surface by the natural secretions of the eccrine glands located in the dermis of the hands and feet. These invisible traces, which contain endogenous and exogenous components of inorganic and organic structures, can be made visible with various chemical reagents. Developed fingerprints allow for physical identification, DNA profiling, and the extraction of chemical content from the trace using advanced spectroscopic methods, yielding more in-depth information.[1]

In criminalistic investigations, latent fingerprints on porous materials (paper and derivatives) are made visible through the Ninhydrin reaction. The resulting traces appear in various shades of purple (Ruhemann's purple). However, to observe traces on dark-colored materials, applications such as DFO (1,8-diazafluoren-9-one), 1,2-indandione, and 5-MTN (5-methylthioninhydrin)/$ZnCl_2$, which have fluorescent properties, are used. The resulting traces can be photographed and studied by taking advantage of the contrast difference. [2-4]

Fluorescent organic substances cover a wide range of studies in literature. Designing substituted ninhydrin reagents with reactions using molecules with high fluorescence yields will enable more effective fingerprinting on dark, porous surfaces. Esterification, substitution, Huisgen [3+2] cycloaddition, and subsequent oxidation reactions (Riley Oxidation by SeO_2) will be used to achieve the most efficient results. Considering the workload of fingerprint laboratories, paper-derived materials, which serve as evidence, hold a significant place. Therefore, chemical studies can be conducted in a more effective, efficient, economical, and environmentally friendly manner. New compound was characterized by FTIR, ^{1}H-NMR, ^{13}C-NMR spectroscopy. Fluorescence properties were investigated by UV–vis spectroscopy and fingerprint laboratory applications.

This research was supported by Yıldız Technical University Scientific Research Projects Coordination Unit with Project Number: FDK-2023-5867.

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The novel LMU-2 zeolite structure and its transition to chabazite

Janina Carolin Höner,[1,2] Andreas Schaate,[1,2,3] Andreas M. Schneider,[1,3] Yaşar Krysiak,[1,4]

[1] *Leibniz University Hannover, Institute of Inorganic Chemistry, Hannover, Germany*
[2] *Hannover School for Nanotechnology, Leibniz University Hannover, Hannover, Germany*
[3] *Cluster of Excellence PhoenixD, Leibniz University Hannover, Hannover, Germany*
[4] *Laboratory for Nano and Quantum Engineering, Leibniz University Hannover, Germany*

Zeolites are nanoporous alumosilicates and have a wide range of applications due to the size and shape of their pores, making them suitable for applications like separations or gas catalysts in organic reactions. They are typically prepared by hydrothermal synthesis using structure directing agents (SDAs) to design the desired pore system. Common SDAs are organic amines or alkylammonium salts. Alternatively, metal complexes can be used, offering the advantage that the metal atom can be incorporated into the framework, thus creating catalytically active centres. However, the use of temperature-stable complexes as SDAs, which can be used as templates for building new catalytically active frameworks and their subsequent calcination have not been systematically investigated.[1]

This work examines the synthesis of a novel zeolitic material, employing the cobalt(III)triazacyclononane (*tacn*) complex as the SDA, which also facilitates the incorporation of cobalt into the framework. Using $[Co(tacn)_2]^{3+}$ cation as SDA in a typical hydrothermal synthesis yields a yellow powder. The crystal structure, so called LMU-2, was determined from 3D electron diffraction (3D ED) and PXRD data, revealing a new zeolite structure with an interrupted silica framework similar to chabazite, with the cobalt complex located inside the major cages. Through 3D ED, more details on the $[Si–O\cdots H\cdots O–Si]^-$ hydrogen position were elucidated. Calcination induces a structural transition into the chabazite framework, studied experimentally using temperature dependent PXRD measurements and Rietveld refinements. This transformation was also accompanied by a colour change to blue, which is attributed to a change in the oxidation and coordination state of cobalt.[1]

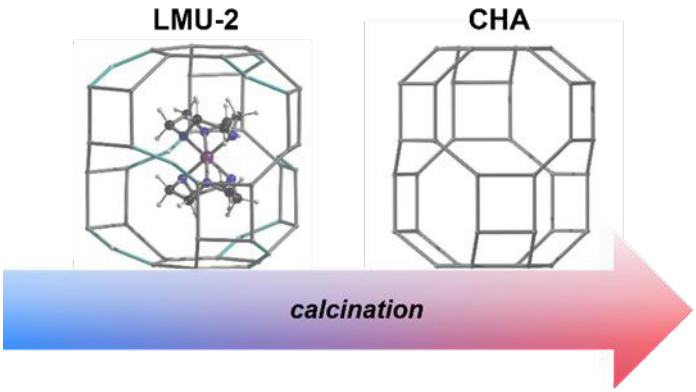

Figure 1: Illustration of structure change from LMU-2 into chabazite.

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P6

Empowering the Next Generation of Chemists: NSYCC Initiatives for Career Development and Community Building

Marcela de Barros[1,2]

[1] *Northeastern Section Younger Chemists Committee, MA, USA*
[2] *Northeastern University, Department of Chemistry and Chemical Biology, MA, USA*

The Northeastern Section Younger Chemists Committee (NSYCC) empowers early-career scientists in the Greater Boston (USA) area by creating spaces where students and professionals can learn, connect, and grow together. Our initiatives focus on helping chemists explore career possibilities, gain presentation experience, and build meaningful networks that extend beyond the lab.

As a means to connect and prepare our members for their professional endeavors, we offer a range of opportunities that comprehend career focus events and opportunities to engage and connect with a range of professionals in our Northeastern Section of the ACS (NESACS) and partnering companies/institutions.



Figure 1: 25th Annual Northeast Student Chemistry Research Conference (NSCRC) at Northeastern University.

Through our Career Symposium, we host panels featuring chemists from a wide range of paths: academia, industry, government, and science communication. This allows attendees to engage directly with professionals who share their experiences and advice. Our Research Student Conference provides an affordable yet scientifically rigorous platform for students to present their work and exchange ideas. This event continues to grow in inclusiveness and impact; last year, we proudly featured participants ranging from high school students to postdocs.

Beyond scientific programming, NSYCC highlights the importance of community through collaborative and fun networking events, such as Bowling with EWOC (Empowering Women in Organic Chemistry), where chemists connect in a relaxed, welcoming environment, and, a distillery tour, where we explored the art and science of producing alcoholic beverages. Together, these initiatives reflect NSYCC's mission to support the next generation of chemists through mentorship, professional growth, and genuine connection.

Multi-Thermoresponsive LCST-UCST Diblock Copolymers in Water

Karla Heckhäuser,[1] Ulrich Jonas[1]

[1] *University Siegen, Macromolecular Chemistry, Siegen, Germany*

Smart materials that respond through non-covalent, reversible interactions to small environmental changes of external stimuli have been reported over the last four decades. They are increasingly important in applications ranging from biomedicine and drug delivery to soft robotics. Among these, thermoresponsive polymers and hydrogels are particularly interesting due to their ability to undergo reversible changes with temperature shifts.

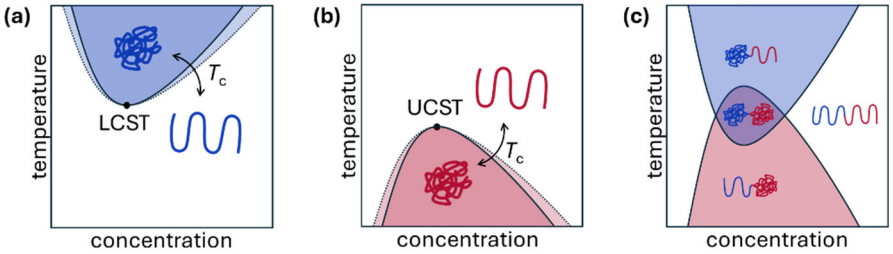

Figure 1: Schematic phase diagrams with temperature against concentration of **(a)** LCST polymers, **(b)** UCST polymers and **(c)** LCST-UCST diblock copolymers.

Thermoresponsive polymers in water show either lower or upper critical solution temperature (LCST/UCST) behaviour. In the phase diagrams (see Fig. 1 **(a)** and **(b)**) each polymer type exists as molecularly dissolved, extended coils in the one-phase regions (white background) because of strong hydrogen bonding between water molecules and the hydrophilic polymer side groups. At the temperature boundary given by the cloud points (T_c) the polymer chains undergo a sharp, reversible transition forming collapsed globules as now hydrophobic interactions of the polymer backbones predominate.

Traditional systems rely on a single thermal response, while recently systems are developed that combine both LCST and UCST behaviors in one block copolymers.[1–3] When combining the complementary parts, a system with two responses is created (see Fig. 1**(c)**). However, systems showing three responses were found. This was attributed to intermolecular influences of one block onto the other. Depending on the solvation state of one block, another environment results for the other block causing a different thermal behaviour. These complex switching systems offer new possibilities for designing highly controllable, multifunctional materials, which are attractive for real-world applications.

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Encapsulated Phase Change Materials in Polypropylene Composites

Elmas Kırtay [1], Tarık Eren [1], Çağatay Elibol [2], Afife B. Hazar Yoruç [3], Kadir Sağır [4], Umutcan Özer [3], Oğuler Sazcı [3]

[1] Yıldız Technical University, Faculty of Art and Science, Chemistry Department Istanbul, Turkiye
[2] University of Technology Chemnitz, Institute of Materials Science and Engineering, Chemnitz, Germany
[3] Yıldız Technical University, Faculty of Chemical and Metallurgical Engineering, Department of Metallurgical and Materials Engineering, Istanbul, Turkiye
[4] Turkish- German University, Faculty of Science Materials Science and Technology, Istanbul, Turkiye

The increasing imbalance between energy supply and demand, along with the growing need for sustainable energy systems, has increased interest in thermal energy storage technologies. In this context, phase change material (PCM)-based thermal energy storage systems offer an effective solution due to their high latent heat capacity and phase transition occurring within a narrow temperature range.[1] [2] However, preventing PCM leakage while maintaining structural stability and adequate thermal conductivity over long-term use remains a critical challenge for practical applications.[3]

In this study, commercially available encapsulated PCM PX-25 (RUBITHERM®) was modified using various surface coating and modification approaches. The effects of surface modification on the dispersion of PCM within a polypropylene (PP) matrix, structural stability, and thermal energy storage behavior were systematically investigated. The modified PCMs were incorporated into the PP matrix via injection molding, and the thermal and structural performance of the resulting PP/PCM composites were evaluated.

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Starch–PAMAM Dendrimer Hybrid Gels for Controlled Urea Release and Sustainable Fertilization

Aylin KAYMAZ[1], Nehir KAYA[1], Mustafa Ulvi GÜRBÜZ[1], Metin TULU[1], Tarık EREN[1]

[1] *Yildiz Technical University, Faculty of Art and Science, Chemistry Departmant Istanbul, Turkiye*

The global population is growing rapidly. This has resulted in a steadily growing demand for food production. Fertilisers play a crucial role in enhancing agricultural productivity, and urea fertiliser is one of the most widely used sources of nitrogen due to its high nitrogen content (46%) and cost-effectiveness.[1] However, urea's low nitrogen use efficiency, coupled with losses through leaching, volatilisation and gaseous emissions, leads to significant economic losses and environmental concerns. Furthermore, repeated application of urea-based fertilisers can negatively impact soil quality.

Starch is a naturally abundant polymer that is biocompatible, biodegradable and highly water-retentive, making it a suitable material for a wide range of applications.[2] The presence of functional groups in its structure means that starch can be easily modified using chemical processes. PAMAM dendrimers are highly biocompatible and have been widely used in biomedical applications. In recent years, there has been growing interest in their potential use in agriculture due to their high nitrogen content.[3,4]

In this study, gel systems with different formulations were prepared using methacrylate-functionalised PAMAM dendrimers and acrylate-functionalised starch polymers. The gels' release behaviour in an aqueous environment was systematically investigated, and their chemical composition, mechanical properties and surface morphology were thoroughly characterised. Additionally, the biodegradation behaviour of the gel systems under soil conditions was evaluated.

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Waste-to-Value: Development of Green and Innovative Materials from Renewable Resources for Boron Adsorption via Photoinduced Inverse Vulcanization

Nazlı KAYA[1], Emrah ÇAKMAKÇI[1]

[1]*Marmara University, Faculty of Science, Chemistry Department, Istanbul, Turkiye*

Elemental sulfur, a major industrial byproduct of petroleum and natural gas processing, represents a substantial environmental burden. This study addresses this by aiming to synthesize environmentally friendly, value-added polymeric materials from two main waste streams: waste sulfur and waste cooking oils. This is achieved through the cross-linking of sulfur with organic components via photoinduced inverse vulcanization (PIV) (Figure 1).[1] The PIV technique, based on the light-energy activation of cyclic sulfur rings, offers a greener and safer alternative by overcoming the high-temperature requirements and H2S gas formation risks associated with classical thermal methods.[2] The resulting high-sulfur content composite materials possess functional properties suitable for the adsorption of boron (B) from aqueous solutions, a contaminant of strategic importance to Turkey.[3] Waste cooking oils were first reacted with glycerol and converted to monoglycerides. Next, the monoglycerides were reacted with elemental sulfur (50:50%) under light irradiation (430 nm) for 6-48 hours. The obtained materials were characterized via Fourier Transform Infrared (FTIR) and proton nuclear magnetic resonance (^{1}H NMR) spectra, as well as thermogravimetric analysis (TGA). The resulting black-brown colored materials have the potential to be used for boron removal from aqueous samples.

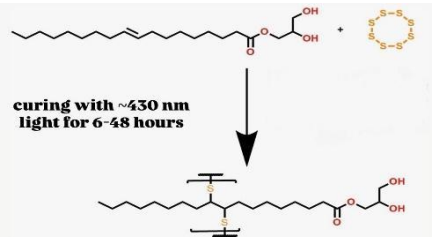

Figure 1: Curing of monoglyceride with sulfur. A monoglyceride containing oleic acid is given as an example

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Enabling activity-based protein profiling (ABPP) for drugs that form disulfides: identification of off-targets for an ALS drug candidate

Durgalakshmi Sivasankar,[1] Wensheng Yang,[1] Brandon Miller,[1] Roman Manetsch,[1] and Jeffrey N Agar[1]

[1] *Department of Chemistry and Chemical Biology, Northeastern University, Boston, USA*

The toxicity of drugs often results from interactions with proteins other than the intended target. Identification of off-targets interactions is therefore a critical step in evaluating potential safety issues for existing and developmental drugs. The stability of the bonds between covalent drugs and their targets presents opportunities and challenges for analytical techniques. Those challenges have been addressed by chemoproteomics techniques for drugs that form carbon-sulfur bonds.[1,2] These techniques, however, cleave disulfide bonds are therefore not applicable to covalent drugs that form sulfur-sulfur bonds. Here we develop a desthiobiotin iodoacetamide (DBIA)-based chemoproteomics methods for the off-target ID of covalent drugs that form disulfides. We apply these to an advanced preclinical candidate for ALS, cyclic thiosulfinate (CT).

A total of 11,215 reactive cysteine residues were profiled from 3,952 protein groups without missing values in a data independent acquisition (DIA) LC-MS/MS experiment with biological replicates (n=3), Fig. 1. Many notable off-target interactions were identified and extrapolated to toxicological effect. In one example, Cys X in target Y (target identity will be disclosed at time of meeting. Currently filing a provisional patent) exhibited significant drug occupancy (93%). Irreversible binding of CT to this site may disrupt the protein's conformation, stability, or lipid droplet association, leading to partial or complete loss of function, even though this cysteine is not a part of the catalytic active site. Such a modification would mimic the protective effects of genetic loss-of-function variants in humans, potentially reducing hepatic lipid accumulation, inflammation, and progression of nonalcoholic steatohepatitis (NASH) and related liver diseases.

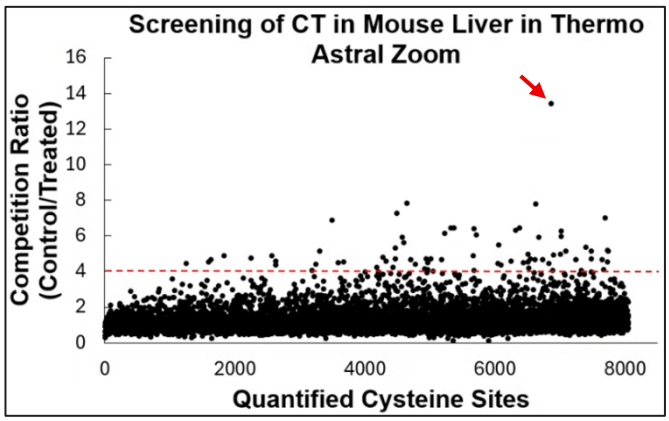

Figure 1: The dotted red line shows the significance threshold (4), which corresponds to 75% drug occupancy. The red arrow highlights an off-target with 93% drug occupancy.

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Plasmon decay pathways in magic sized nanoclusters: Hot-carrier dynamics for photocatalyst design

Anant O. Bhasin,[1] Rebecca L.M. Gieseking,[1] Katherine E. Shulenberger, [1]* George C. Schatz[2]*

[1] *Department of Chemistry, Brandeis University, Waltham, Massachusetts 02453, USA*
[2]*Department of Chemistry, Northwestern University, Evanston, IL 602010, USA*

Plasmonic metal nanoparticles have emerged as powerful materials with application ranging from optoelectronics and photocatalysis, owing to their ability to confine the light at the nanoscale.[1–3] The utility of these materials has arisen from the generation of energetic charge carriers, hot electron and holes.[4] However, plasmon-driven and plasmon-enhanced photocatalysis faces challenges due to the rapid thermalization of hot carriers generated by plasmon decay, significantly impacting their photocatalytic efficiency.[5] In this study, we investigate the decay channels of plasmonic excitations in noble metal nanoclusters using a combination of linear-response and real-time time-dependent density functional theory (TDDFT).[6] We resolve the coupling between plasmonic modes and specific excited-state transitions, identify the role of state mixing and dephasing, and explore how these pathways evolve with the nature of metal. By mapping the electronic response to external fields and analyzing spectral features correlated with specific decay routes, we provide a predictive framework for tailoring plasmonic nanostructures to maximize hot carrier generation and lifetimes. We evaluate how these decay pathways translate to small molecule photocatalysis (e.g., N_2), with particular focus on the role of molecular orientation in governing catalytic activity.

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Characterizing Defects in InP Quantum Dots through Structural and Optical Characterization of InP Magic-sized Clusters

Hannah Lynn Harrison[1], Katherine Shulenberger[†]

[1] *Brandeis University, Department of Chemistry, Waltham, United States*

Indium phosphide (InP) quantum dots (QDs) have become promising candidates for heavy-metal-free light emitting diodes (LEDs)[1,2] and light sources for high-speed fiber optic communication[3]. They are a direct bandgap (bulk: 1.35 eV) III-V semiconductor with tailorable emission ranging across the visible spectrum (~1.3 eV to ~3 eV) and high carrier mobility. While InP QDs are promising alternatives to heavy metal containing cadmium chalcogenides, the more covalent nature of the lattice requires substantially more reactive precursors which limit synthetic control and make these nanocrystals extremely prone to lattice defects. As commercial applications such as white-light LEDs require precise controllable photoluminescent emission lines and high emission quantum yields, the broad emission profile created by poor synthetic size control has detrimental impacts on device performance.[1] While lattice and surface defects are crucial to the generation of broad-spectrum white-light emission in InP QDs[4], the structure and optical properties of these defects are not well understood. To advance understanding and control of defects in InP QDs, suite of 2D ^{31}P and ^{1}H NMR techniques were used to structurally characterize InP magic-sized clusters ($In_{37}P_{20}$, $In_{26}P_{13}$, and F_{360}-InP) across an array of surface ligands in parallel with optical characterization using static and time-resolved absorption and emission spectroscopies. The changes in surface structure and the resultant emergence of trap states in the magic-sized cluster can then be extrapolated to optical behavior exhibited in InP QDs. Identification and sourcing of these defects will permit focused development of synthetic methodologies and post-synthetic remedy or induction of defects.

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Predicting the Stability of Base-mediated C–H Carboxylation Adducts Using Data Science Tools

Maike Eckhoff,[1,2] Shubham Deolka,[2] Aleria Garcia-Roca,[2] Lilly Meynberg,[1] Liudmila Seidel,[1] Matthew S. Sigman,[2] and Jonny Proppe[1]

[1] *TU Braunschweig, Institute of Physical and Theoretical Chemistry, Braunschweig, Germany*

[2] *University of Utah, Department of Chemistry, Salt Lake City, United States*

Using CO_2 as a direct C1 building block is a powerful strategy for making new molecules,[1] especially when reactions can run under mild, transition-metal-free conditions such as in C–H carboxylation.[2] However, many promising approaches fail because the resulting CO_2 adducts are often insufficiently stable.[3]

Here, we introduce a predictive data-driven workflow (Fig. 1) to address this limitation.[3] By combining density functional theory with multivariate linear regression (MLR), we establish a quantitative framework to assess CO_2 adduct stability prior to experimental testing.[3] Our MLR model is based on three simple, physically interpretable parameters that capture electronic and steric effects.[3]

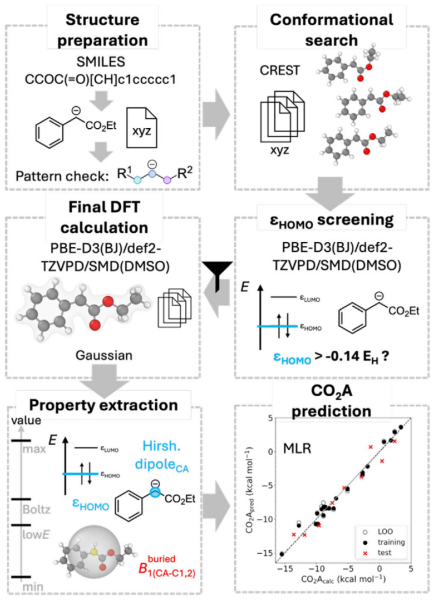

Figure 1: Workflow steps involved in the automated predictions of CO_2 affinities.[3]

We demonstrate the utility of this approach by screening 60 previously unexplored nucleophiles.[3] Our MLR model reliably differentiates between stable and unstable CO_2 adducts, as confirmed by experimental validation.[3] Overall, this works illustrates how data-driven modeling can move CO_2 chemistry beyond trial-and-error, providing a rational roadmap for identifying suitable substrates for successful C–H carboxylation.[3]

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P15

Investigation of Thermodynamic Properties of White Benzoin by Inverse Gas Chromatography Method

Ayse ERDOGAN CAKAR,[1] Hatice Kubra ERDOGAN[1]

[1] *Yildiz Technical University, Chemistry Department, Istanbul, Turkiye*

Benzoin, produced from the styrax tree native to South Asian countries such as Indonesia, Thailand, and Sumatra, is a resin widely used in therapeutic and cosmetic fields. Structurally, it consists of benzoic acid, conephyl benzoate, cinnamic acid, and various triterpenoids. The ratio of its components varies depending on the type [1].

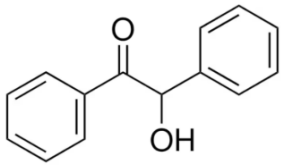

Figure 1: Chemical structure of benzoin

Inverse gas chromatography (IGC), a highly sensitive characterization technique, is a cost-effective and simple method. Unlike conventional gas chromatography, IGC uses a stationary phase to analyze high molecular weight materials placed in a chromatographic column. Various solvents with specific properties are injected into the column as the mobile phase. With the help of the retention time of the solvent, whose properties are known, in the substance to be analyzed, various physical and chemical properties of the substance can be determined [2].

The IGC method was used to determine the thermodynamic properties of the white benzoin-solvent system. For this purpose, retention diagrams were plotted using the interactions between white benzoin and carefully selected solvents between 100 and 125 ℃. The white benzoin-solvent interaction parameters for the Flory-Huggins parameter, equation of state interaction parameter, mole fraction activity coefficient, effective exchange energy parameter, and residual thermodynamic parameters were calculated between 100 and 125 ℃.

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Diels-Alder-Based Thermoreversible Silicone Networks

Sophie Wagner,[1] Malte Kunz,[1] Esteban Mejia,[1]

[1] *Leibniz Institute for Catalysis at the University of Rostock (LIKAT), Rostock, Germany*

Silicones are inorganic polymers featuring a silicon-oxygen backbone. Depending on their polymeric architecture, they are employed in a wide range of applications.[1] However, due to their chemical inertness and significant carbon footprint,[2] increasing research efforts are focused on recycling and reuse strategies. In this context, debonding-on-demand represents a key approach to mitigating silicone-derived polymeric pollution. In this study, Diels-Alder chemistry is employed to construct reversible silicone networks. A library of silicone-based dienes and dienophiles was synthesized as network precursors. Previously reported silicone-based furan/maleimide systems[3] were expanded by introducing thiophenes as alternative diene partners for bismaleimides. Attachment of both the diene and dienophile functionalities to silicone chains was achieved via hydrosilylation reactions, with bismaleimides serving as the crosslinking agents. The Diels-Alder reaction is characterized by adduct formation at lower temperatures and thermal reversibility at elevated temperatures, enabling the development of self-healing polymer networks.[2] Reaction optimization revealed that both the [4+2] cycloaddition and the retro-[4+2] cycloaddition of thiophene-based systems require higher temperatures compared to their furan analogues. Overall, reversible thiophene-bismaleimide silicone systems were successfully shown to form crosslinked silicone networks, enabling higher-temperature applications while retaining debonding-on-demand functionality.

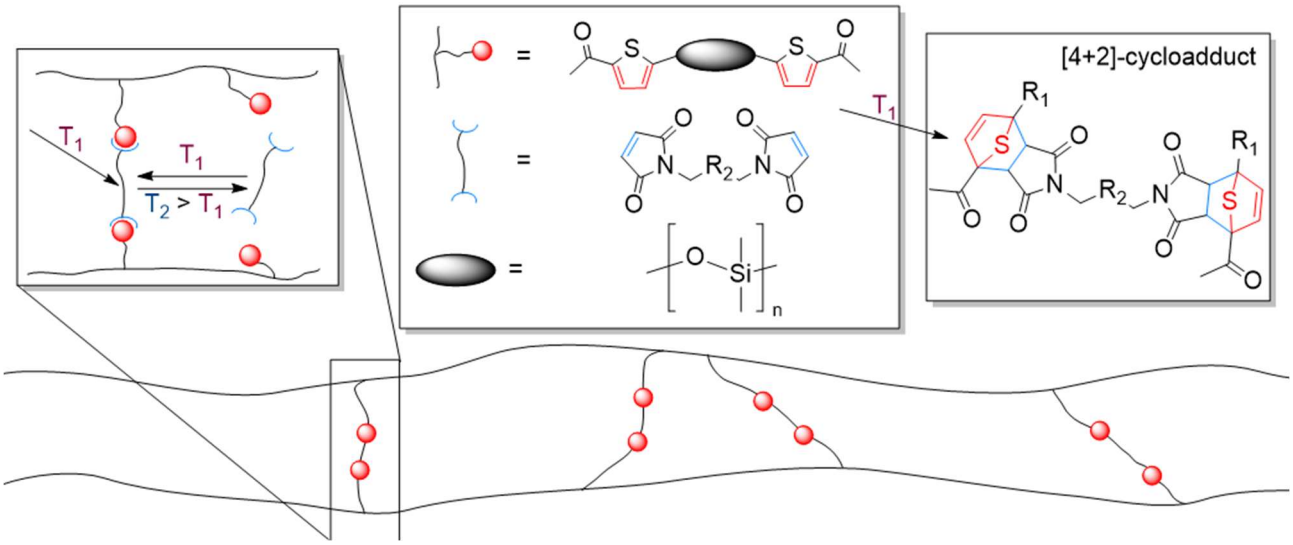

Figure 1: Schematic figure of a Diels-Alder crosslinked silicone network.

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P17

Synthesis and Characterization of Novel Thienyl-Methylene Substituted 1,3-Thiazolidinone Derivatives

Ömer Tuğcu, Fatma Tülay Tuğcu[1]

[1] *Yildiz Technical University, Faculty of Science, Department of Chemistry, İstanbul, Türkiye*

The Iminothiazolidinone core is a well-known heterocyclic scaffold that has been extensively investigated due to its versatile chemical reactivity and promising biological relevance [1–3]. Structural modification of this nucleus through variation of aromatic substituents and heteroaryl moieties represents an effective strategy for the development of novel functional molecules [4]. In this study, the synthesis and structural characterization of four new thienyl-methylene-substituted 1,3-thiazolidinone derivatives bearing different aromatic imino groups are reported.

The structures of the synthesized compounds were elucidated using IR, ^{1}H NMR, and ^{13}C NMR spectroscopic techniques. The characteristic absorption bands and resonance signals corresponding to the carbonyl, imine, and thiazolidinone ring system confirmed the successful formation of the target molecules. The influence of methyl- and chloro-substituted aromatic rings on the spectral features was also observed, indicating substituent-dependent electronic effects.

The newly synthesized thienyl-methylene-substituted iminothiazolidinone derivatives expand the structural diversity of the 1,3-thiazolidinone family and may serve as potential candidates for further biological activity and structure–activity relationship studies.This study introduces new thienyl-methylene-substituted iminothiazolidinone derivatives to the literature. The synthesized compounds are considered promising candidates for further investigations focusing on their biological activities and structure–activity relationships.

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P18

The HyDRA blind challenge on microhydration: past, present and future

Margarethe Bödecker,[1] Martin A. Suhm[1]

[1] *Georg-August University, Institute of Physical Chemistry, Göttingen, Germany*

The field of gas phase spectroscopy benefits from a robust interplay between quantum chemistry and experimental techniques. However, the vast array of available quantum chemical methods, coupled with the inherent limitations of experimental approaches, can lead to fortuitous and biased matches, particularly when the experimental outcome is known in advance. To facilitate the advancement of systematically enhanced quantum chemical predictions in vibrational spectroscopy and solvation science, we have organized the HyDRA (Hydrate Donor Red Shift Anticipation) blind challenge during the 2021/22 academic year within the framework of the DFG research training group BENCh.[1]

In this challenge, ten cold 1:1 complexes of organic molecules with water were prepared in a vacuum and examined by infrared and Raman spectroscopy for the first time. The fundamental vibration of the hydrogen-bonded water molecule (OH stretching) in these complexes was measured and kept secret until ten interested theoretical research groups worldwide had made their predictions in spring 2022. The detection of a robust anharmonic resonance in some of these water complexes[2] rendered this competition not only interesting for scaled harmonic predictions, but also for more elaborate anharmonic treatments.

This contribution describes the blind challenge from an experimental perspective and presents a survey on the performance of the various theory submissions.[3] An outline of the aim and focus of the second round of the HyDRA blind challenge (2025/2026) will be given.

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P19

Synthesis and characterisation of amphiphilic, metal-containing block copolymers via anionic polymerization

Kathrin Kolling, Markus Gallei

Saarland University, Chair of Polymer Chemistry & Saarene, Saarland Center for Energy Materials and Sustainability, Saarbrücken, Germany

Amphiphilic block copolymers (BCPs) composed of immiscible segments can self-assemble in the bulk state into ordered nanostructures such as spheres, cylinders, and lamellae.[1] Owing to their periodic domain structures, BCPs are widely used in applications including ordered porous materials, lithographic templates, and photonic band-gap materials.[2] Ferrocene-containing BCPs exhibit high thermal and chemical stability alongside useful electrical properties, making them suitable for applications ranging from ceramic precursors to biomedical and sensing materials. Although ferrocene polymers were first reported in 1955[3], significant progress occurred in 1992 with the discovery of 1,1′-dimethylsilaferrocenophane, enabling ring-opening polymerisation and access to well-defined, high-molar-mass polymers.[4] Since then, polydimethylsilaferrocenophane (PFS)-based BCPs have attracted considerable interest due to their etch resistance, catalytic and redox activity, and ability to form magnetic ceramic nanodomains.[5] Polylactic acid (PLA) is produced either by condensation polymerisation of lactic acid or by tin(II)-catalysed ring-opening polymerisation (ROP) of lactide. Its versatility in applications such as 3D printing, coatings, and packaging, combined with its renewable origin, makes PLA an important material for sustainable technologies.[6] This study presents the synthetic route to well-defined PFS-*b*-PLA BCPs. Endfunctionalisation of PFS was achieved through the end capping of active carbanionic PFS chains with benzyl glycidyl ether (BGE). The monohydroxyl-functionalised PFS obtained is then used as a macro-initiator for the catalytic ROP of *L*-lactide. This route offers a convenient way of fabricating nanoporous materials by using the capability of selective degradation of the PLA block segment. A range of BCPs were synthesised with varied PLA chain length and characterised by ^{1}H NMR spectroscopy, size exclusion chromatography (SEC), differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). Furthermore, self-assembly behaviour of the polymers in THF and chloroform was investigated. To characterise the resulting morphology, ultrathin films were prepared and transmission electron microscopy (TEM) was performed.

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Novel Furan Ring-Based Rod-Shaped Molecules: Synthesis, Characterization and Investigation of Mesomorphic Properties

Ceren Can Karanlık,[1] Barış Sezgin,[2] Gürkan Karanlık[1]

[1] *Yildiz Technical University, Department of Chemistry, Davutpaşa Campus, 34220, Esenler, Istanbul, Turkey*

[2] *Süleyman Demirel University, Department of Chemistry, 32260, Cunur, Isparta, Turkey*

Liquid crystals (LCs), which possess characteristics of both solid crystals and isotropic liquids, are self-organized advanced functional materials. Due to their extraordinary physical and chemical properties, LCs have a wide range of application areas such as LCDs, DSSCs, OLEDs, LC-based sensors, drug delivery systems, imaging and diagnostics. In addition, recent advancements have yielded deeper insights into liquid crystalline systems, thereby enabling the rational design, optimization, and functionalization of liquid crystalline materials.[1]

Calamitic LCs are characterized by their linear rod-shaped geometry, and they consist of rigid aromatic cores and flexible terminal chains. Linking groups such as ester, imine, and azo moieties between rings help to keep linearity, increase flexibility and provide mesophase stability and diversity.[2] Additionally, the introduction of heteroatom or heterocycles such as furan, pyrrole, and thiophene as molecular building blocks into the core structures of the mesogens influence mesophase behaviour by altering polarity, polarizability and dipolar interactions both lateral or longitudinal, enabling interesting optical and thermal features.[3,4]

In this study, the synthesis, structural and mesomorphic characterization of two novel thermotropic rod-shaped liquid crystalline molecules based on furan-ring connected with chalcone/ester/ester or chalcone/ester/azo linkages are presented. The liquid crystalline properties of the molecules were evaluated by polarized optical microscopy (POM) and differential scanning calorimetry (DSC). The results indicated that both mesogens displayed enantiotropic smectic A (SmA) phases, while the azo-linked molecule additionally revealed a monotropic nematic phase (N) upon cooling. Also, photoisomerization studies under UV irradiation showed the reversible trans-cis transformation of the azo-linked mesogen, demonstrating its potential in light-responsive systems. This work underlines how the minor alterations in the molecular architecture such as the nature of the linking units can significantly affect the thermal, photoresponsive and mesomorphic properties of liquid crystals.

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A 100,000-Fold Increase in C-H Bond Acidity Gives Palladium a Key Advantage in C(sp^3)-H Activation Compared to Nickel

Lirong Lin,[1†] Tim K. Schramm,[2†] Pavel Kucheryavy,[1] Roger A. Lalancette,[1] Andreas Hansen,[2*] and Demyan E. Prokopchuk[1]

[1] Rutgers University-Newark, Department of Chemistry, Newark, New Jersey, USA
[2] Rheinische Friedrich-Wilhelms Universität Bonn, Mulliken Center for Theoretical Chemistry, Clausius-Institut für Physikalische und Theoretische Chemie, Bonn, Germany

This work presents a comprehensive computational and experimental investigation into the striking differences in C(sp^3)-H bond activation as a function of transition metal identity. Using experimental insights and a multi-level workflow combining state-of-the-art density functional theory calculations, we demonstrate that C(sp^3)-H bonds coordinated to palladium are acidified by approximately five pKa units (~10^5-fold increase in acidity) compared to their nickel counterparts. Further, beyond mere thermodynamic changes, our calculations show that this acidification may also have kinetic implications, as manifested in markedly different potential energy surfaces for C(sp^3)-H activation pathways with palladium versus nickel catalysts.

We employed extensive conformational sampling via CREST [2] and GOAT [3], with particular attention on the non-covalently bound adducts to model the complex solution-phase dynamics underlying the experimentally measured (ion) equilibria. Default sampling parameters proved insufficient for these challenging systems, requiring modifications to the settings of the NCI workflow in CREST, such as a reduced meta-dynamics temperature and a tighter wall potential. These adjustments highlight the need for an automated NCI parameter adjustment procedure to handle diverse chemical systems in future computational studies efficiently.

Thus, we show how computational analysis can provide fundamental insights into metal-specific reactivity patterns while critically reflecting on the computational methodologies employed, revealing the need for further improvements.

† L.L. and T.K.S. contributed equally to this work.

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Young Chemists Network (JCF) Ulm

Irene Boeck [1]

[1] *University of Ulm, Young Chemists Network, Ulm, Germany*

The Regional Young Chemists Network of Ulm is an active association of bachelor's and master's students as well as doctoral candidates in chemistry and related fields. We meet monthly to discuss relevant topics and to organize upcoming events, followed by a social networking session including food and board games.

At least once per semester, we organize scientific talks featuring invited speakers from various thematical fields. We regularly cooperate with the student body of the chemical studies and contribute to their summer party as well as participate in their introductory week for first-semester students. In addition, we take part in the Long Night of Science of the University of Ulm with the ChemEscape kit provided by the JCF Team Science and Education.

During the past summer semester, we arranged a dodgeball tournament for chemistry students and doctoral candidates.

In 2024, we hosted the Spring Symposium which was jointly organized with JCF Stuttgart and JCF Munich.



Figure 1: “Meet Your Prof”- talk with Prof. Dr. Sabine Richert and Prof. Dr. Simon Krause (top left). JCF Ulm at the dodgeball tournament in June 2025 (top right). The organizing team of the Spring Symposium 2024 in Ulm (bottom).

OH NO! – The microsolvation of TEMPO derivatives in the gas phase

Elisabeth Sennert,[1] Dana Donnerstag,[1] Martin A. Suhm[1]

[1] *Georg-August-Universität, Institut für Physikalische Chemie, Göttingen, Germany*

In line with the conference theme, many radicals exhibit colourful chemistry due to their unpaired electrons. This also applies to aminoxyl radicals, such as TEMPO, TEMPONE, and TEMPOL (Fig. 1), which are investigated in this work. Brás *et al.* conducted the first studies on the microsolvation of TEMPO in the gas phase, investigating clusters of TEMPO with water and smaller alcohols.[1,2] The present work builds on these previous investigations by incorporating TEMPO derivatives and larger alcohols. Due to the formation of a hydrogen bond between the radicals and the alcohols, the OH stretching vibration of the alcohol can be used as a sensitive probe for the presence of a specific heterodimer (1:1) conformation by comparing slit jet FTIR spectra with the results of harmonic DFT calculations. The conditions of the cold, isolated gas phase make the generated experimental data highly suitable for the benchmarking of theoretical methods.

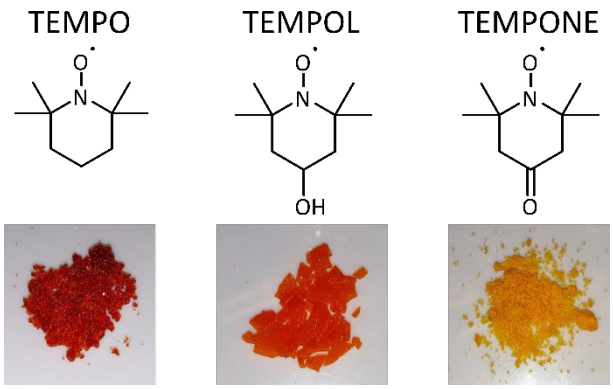

Figure 1: The diverse colour palette of the investigated TEMPO derivatives.

The pairing of TEMPO with benzyl alcohol and its halogenated derivatives exhibits two main conformers with different ring-stacking behaviour. The preference for one of these conformers can be controlled by introducing halogen atoms at different positions of the alcohols aromatic system.[3,4] Increasing conformer diversity was found for the clusters of TEMPONE with benzyl alcohol because the CO group of TEMPONE can act as an additional hydrogen bonding site.[4] For TEMPOL, which includes an OH group at the *para*-position, the self-aggregation was investigated.[5]

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Mechanochemical room-temperature synthesis of C_2N-type materials from HATCN and its precursors

Pascal Dippner[1], Sven Grätz[1], Lars Borchardt[1]

[1] *Ruhr University Bochum, Institute of inorganic chemistry I, Bochum, Germany*

Carbon materials have attracted growing interest as zeolite-like adsorbents and catalysts for environmental and energy-related applications.[1] Their properties can be tailored by incorporating nitrogen, for example through the use of nitrogen-rich precursors.[2] Hexaazatriphenylenehexacarbonitrile (HAT-CN) is a well-established precursor for nitrogen-rich carbons with C_2N-type structure, typically obtained by energy-intensive thermal treatment.[3] Herein, we report a mechanochemical one-pot synthesis of C_2N-type materials under ambient conditions as a greener alternative to conventional pyrolysis. Using HAT-CN, systematic variation of milling parameters enabled reaction optimization and revealed the decisive role of mechanical energy in directing framework formation, achieving yields above 80 %.

In addition, C_2N-type materials were directly synthesized from the HAT-CN precursors hexaketocyclohexane and diaminomaleonitrile via mechanochemical treatment, bypassing the need to synthesize, purchase or isolate HAT-CN itself entirely. A comparative green metrics analysis confirms the significantly improved sustainability of both mechanochemical routes, primarily due to their drastically reduced energy consumption.

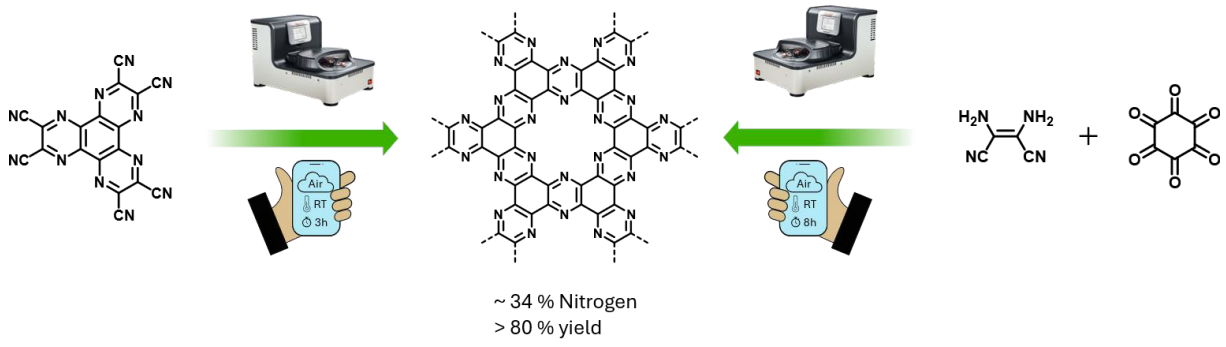

Figure 1: The mechanochemical synthesis of C_2N-type materials under ambient conditions.

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Temperature-Triggered Depolymerization of Dilution-Resistant Supramolecular Polymer Bottlebrushes

Alina Kasberg,[1] Lisa Günther,[2] Johannes C. Brendel [1]

[1] *University of Bayreuth, Macromolecular Chemistry I, Bayreuth, Germany*
[2] *University of Bayreuth, Spectroscopy of Soft Matter Group, Bayreuth, Germany*

Supramolecular self-assembly into anisotropic structures is a recurring phenomenon in nature exemplified by the cytoskeleton of cells composed of microtubules and actin filaments. In recent years, synthetic approaches attempting to mimic these systems have led to interesting supramolecular fibers including macromolecular building blocks forming supramolecular polymer bottlebrushes (SPBs). We have recently developed a benzenetrispeptide motif that enables versatile modifications of the amino acid groups or attachment of various polymers while still forming stable SPBs. Under ambient conditions, the SPBs are non-dynamic revealing no exchange of building blocks. However, heating can trigger dynamic behaviour of the SPB. To further explore these properties, we examined SPBs at nanomolar concentrations across temperatures ranging from 8 °C to 80 °C using fluorescence correlation spectroscopy (FCS). This approach allowed us to determine the critical concentration and elucidate the mechanism of supramolecular polymerisation.

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Control of self-assembly of supramolecular polymer bottle brushes based on benzene tripeptides via microfluidics

Alina Kasberg,[1] Johanna Koll,[1] Johannes C. Brendel[1]

[1] *University of Bayreuth, Macromolecular Chemistry I, Germany*

Supramolecular self-assembly into anisotropic structures is a recurring phenomenon in nature. Examples are the cytoskeleton of cells, which consists of microtubules and actin filaments or collagen fibers. In recent years, synthetic approaches attempting to mimic these systems have led to interesting supramolecular fibers including macromolecular building blocks forming supramolecular polymer bottlebrushes (SPBs). We have recently developed a benzenetrispeptide motif that allows versatile modifications on the amino acid groups or attachment of various polymers forming stable SPBs. Interestingly, the preparation method appears to have a tremendous influence on the self-assembly of these materials. In a recent attempt, we try to gain improved control over the process using microfluidics and investigate different assembly pathways using various microfluidics chips. Thereby, we compared a chip based on only molecular diffusion and a chip based on molecular diffusion and passive mixing due to herring bone shape channels. This analysis enabled us to control the length and distribution of the SPBs between few nanometers and several micrometers.

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Functionalized Initiators for Anionic Polymerization: Investigating the Relationship between Structure and Reactivity in Ethers

Thokozire E. Sweetland,[1] Prof. Dr. Carsten Strohmann[1]

[1]*TU Dortmund University, Department of Inorganic Chemistry, Dortmund, Germany*

Living anionic polymerization enables the precise preparation of polymers with chain-end functionalization, which can form more complex polymer architectures, such as block copolymers and star polymers. Organolithium compounds are commonly used as initiators for living anionic polymerization and can be modified to realize α-chain-end functionalization.[1,2]

In this work, the reactivity of functionalized organolithium initiators was explored through the model initiation reaction with 1,1-diphenylethylene (**1**) and was observed under varying reaction conditions (solvent, temperature, and time). Although a variety of functionalized initiators were tested, only fluorenyllithium, its 9-methyl derivative, and an organolithium phosphine showed reactivity under these conditions.

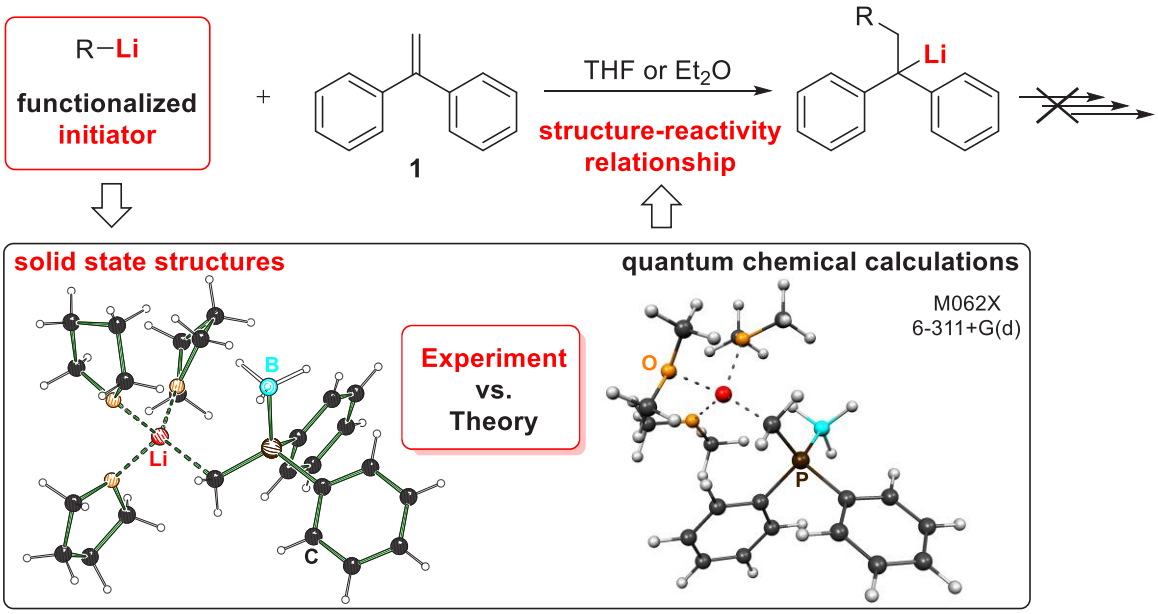

Figure 1: Comparison between the DFT calculations and the experimental data in THF and DME.

Solid-state structures of these functionalized initiators, obtained in THF, revealed the stabilization of the carbanion through *π*-systems or *α*-heteroatoms, which likely influenced the reactivity of each carbanion towards **1**. Analogous solid-state structures obtained with dimethyl ether were used to evaluate the use of DME as an approximation for other ethers in quantum chemical calculations. It was found that the most important structural characteristics were conserved in quantum mechanical calculations when DME was used as an approximation for THF.

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Reactivity of Platina(II)pnictinidenes with Maleic Anhydride

Nils Wegerich[1], Marc. C. Neben[2], Sven Schneider[2], Max C. Holthausen[1]

[1]*Goethe University, Institute of Inorganic and Analytical Chemistry, Frankfurt, Germany*
[2]*Georg August University, Institute of Inorganic Chemistry, Göttingen, Germany*

Pnictinidenes (**Pn**–R; Pn = N-Bi) are subvalent and therefore highly reactive pnictogen compounds possessing only six valence electrons. Depending on the Pn atom and its chemical environment, they feature a triplet or a (multi-reference) singlet ground state.[1-3] In both cases, the two π(Pn) orbitals are (formally) singly occupied in addition to a σ lone pair at Pn. Consequently, pnictinidenes might exhibit reactivity patterns as electrophiles, as radicals, and as nucleophiles. While the diradical reactivity of organic triplet nitrenes (**N**–R) is broadly established, for example in cycloaddition and C–H insertion reactions, examples for nucleophilic reactions are reported far less frequently.[4] In contrast, reactivity studies of their heavier analogues like phosphinidenes (**P**–R) are scarce.[5]

We herein report a quantum chemical mechanistic study of the reactions of a triplet platina(II)nitrene $^{N}\mathbf{2}_{T}$ and -phosphinidene $^{P}\mathbf{2}_{T}$ with maleic anhydride. The pnictinidenes $^{Pn}\mathbf{2}_{T}$ were experimentally generated *in-situ* by photochemical dissociation of precursors $^{Pn}\mathbf{1}$ in toluene (*Figure 1*). While the phosphinidene reacts as a classical diradical via C=C cycloaddition to form phosphirane $^{P}\mathbf{4}_{CS}$, the nitrene inserts in one of the bridging C–O bonds to form 1,2-oxazine-like $^{N}\mathbf{3}_{CS}$. A quantum chemical study of the reaction pathways is presented and detailed analyses relate the electronic structure of key intermediates with their reactivity.

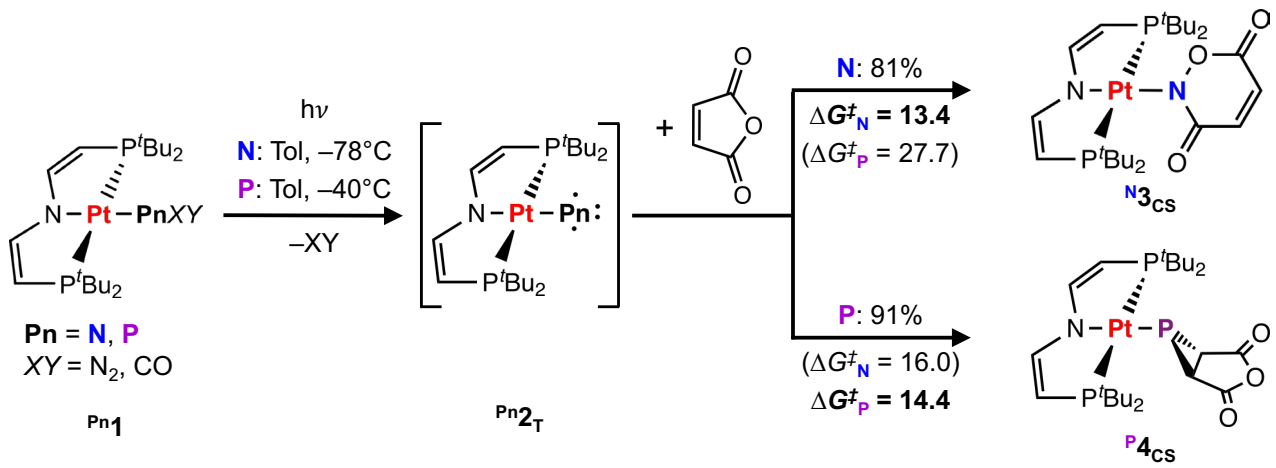

Figure 1: Photochemical generation of pnictinidenes $^{Pn}2$ and subsequent reaction with maleic anhydride to $^{N}3_{CS}$ and $^{P}4_{CS}$. Reaction barriers ΔG‡ in kcal mol^{-1}; Pn = N: $\Delta G^{195\,K}$; Pn = P: $\Delta G^{233\,K}$.

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Gas meets Solid – Gas-mechanochemistry for catalytic reactions

Maike Mayer,[1] Maximilian Wohlgemuth,[1] Lars Borchardt[1]

[1] *Ruhr-University, Inorganic Chemistry I, Bochum, Germany*

The direct reaction of gaseous and solid substrates remains a challenge in chemistry. Commonly, reactions between such substrates are circumvented by dissolving solids in a solvent. However, this approach has significant limitations; dissolution introduces mass transfer barriers and solubility constraints. These challenges are especially pronounced in catalytic processes, where the transport of gaseous substrates to solid catalyst surfaces often becomes rate-limiting. We present an alternative path for the reaction of gases and solids: Gas-Mechanochemistry. Ball milling facilitates contact between gaseous and solid phases and drives the reaction using mechanical impact. As such, solubility- and diffusion-limitations are bypassed in a solvent-free system. Using a catalyst incorporated in the milling material, these reactions allow for simple catalyst recovery and reuse. Based on this, we have established protocols for various ligand-free reduction and oxidation reactions. Selective hydrogenation of a multitude of functional groups and reductive amination proceed under mild conditions, achieving turnover numbers and frequencies several orders of magnitude higher than conventional heterogeneous systems.[1] Furthermore, we demonstrate that atmospheric oxygen suffices as an oxidant for the selective oxidation of alcohols to aldehydes, again with exceptional catalytic performance.[2] As emphasized by these examples, mechanochemistry provides a versatile tool for gas-solid reactions, enabling atom-efficient transformations.



Figure 1: *Left:* Schematic representation of the milling vessel used for gas-mechanochemistry with incorporated catalyst. *Right:* Photograph of the milling vessel with incorporated palladium layer.

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Alkylthio aurone fluorophores: a structure–property relationship of emission in solution and in the solid state

Sören Steup,[1] Sergey Druzhinin,[2] Dieter Schollmeyer,[3] Daria V. Berdnikova [1]

[1] *Universität Siegen, Organische Chemie II, Siegen, Germany*
[2] *Universität Siegen, Physikalische Chemie I, Siegen, Germany*
[3] *Johannes-Gutenberg-Universität Mainz, Institut für Organische Chemie, Mainz, Germany*

The design of solution- and solid-state emitters (SSSE) attracted significant interest in recent years because of fascinating photophysical properties of this type of fluorophores.[1,2] For example, the same SSSE fluorophore can be used in both diluted solutions and in an aggregated/solid state, with no loss of emission. This means that there is no need to adjust the molecular structure for a specific purpose.

In this study, we identify molecular design strategies allowing to construct SSSE fluorophores with controllable properties, based on aurones as an easily accessible scaffold for fluorescence in the solid or aggregated state.[3] To achieve this goal, we performed design and synthesis of five alkylthio aurone derivatives comprising methyl, *n*-propyl, isopropyl, cyclohexyl, and *n*-octyl substituents at the 4'-S atom of the phenyl ring. To establish the structure–property relationships of the alkylthio aurones, we investigated their photophysical properties in solution and in the solid state using steady-state and time-resolved optical spectroscopy methods as well as single crystal X-ray diffraction analysis.

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Fabrication and characterization of a hydroxyapatite-containing biodegradable polymer composite

Karolina Trojanowska,[1] Mirosława El Fray,[1] Agata Goszczyńska[1]

[1] *West Pomeranian University of Technology in Szczecin, Department of Polymer and Biomaterials Science, Faculty of Chemical Technology and Engineering, Szczecin, Poland*

Bioactive polymer composites combine a load-bearing polymer matrix with a dispersed mineral phase. This combination enhances material–tissue contact and can trigger the formation of an apatite-like layer. Therefore, such composites are considered for scaffolds and fillers for bone defects in orthopedics and dentistry. Mineral fillers, especially calcium phosphates, provide bioactivity and osteoconductivity by supporting bone ingrowth and promoting mineral deposition on the material surface. A representative filler is hydroxyapatite (HA) with a Ca/P molar ratio of ~1.67.[1]

The polymer matrix is the continuous phase that carries the applied load and transfers stress to the dispersed HA phase through the polymer-filler interface. It also ensures structural integrity and can be designed to provide hydrolytic stability or controlled degradation, depending on the application and environment. PBF-DLF is a biobased copolyester composed of rigid segments derived from ester derivatives of 2,5-furandicarboxylic acid and flexible segments derived from fatty acid dimers. The rigid-to-flexible segment ratio and the overall crystallinity (primarily associated with the rigid segments) govern the mechanical and thermal performance, while the presence of ester bonds makes the copolyester susceptible to hydrolytic degradation.[2] Owing to its good melt processability, PBF-DLF is a suitable matrix for polymer-ceramic composites, enabling homogeneous HA dispersion, promoting interfacial adhesion, and allowing property tailoring.

In this work, PBF-DLF/HA composites with a rigid-to-flexible segment ratio of 50/50 wt.% and HA contents of 10 and 20 wt.% were manufactured by extrusion. Physicochemical characterization included evaluation of microstructure and filler dispersion, as well as mechanical and thermal testing. Bioactivity after exposure to simulated body fluid (SBF) was assessed by surface morphology analysis with emphasis on apatite-like layer formation. These results provide a basis for assessing how HA content affects the structure-property relationships of PBF-DLF composites and their potential in bone-contact applications.

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Solid State Synthesis of Quantum Dots and Investigation of Dye Adsorption Properties for Waste Treatment

Elif Çeltek,[1] Caner Ünlü,[2]

[1] *Istanbul Technical University, Department of Chemistry, Istanbul, Turkey*
[2] *Istanbul Technical University, Department of Chemistry, Istanbul, Turkey*

In this study, the solid-state synthesis and characterisation of Cu/In/Se ZnS quantum dots (QDs) are discussed. The synthesis was conducted via a one-pot, two-stage process using a stabilizer, and key parameters such as reaction temperature, solution pH, precursor concentrations, feed rates, and shell coating time were optimized.[1] The effect of surface chemistry on particle properties was investigated by using N-acetyl-L-cysteine (NAC), 3-mercaptopropionic acid (3-MPA), and L-glutathione as alternative capping agents during synthesis. Following the synthesis process, structural and surface characterizations were performed to understand ligand-nanocrystal interactions. The functional groups and surface characteristics of the synthesized QDs were examined using Fourier-Transform Infrared (FTIR) Spectroscopy and X-Ray Diffraction (XRD).

The structural and chemical insights gained from these characterizations highlight the potential of these QDs as outstanding solutions for environmental waste treatment, primarily due to their unique nanoscale characteristics and quantum confinement effects.[2] In this study, the environmental remediation potential of synthesised Cu-In-Se-based QDs was evaluated by examining their photophysical properties via UV-Vis and Photoluminescence Spectroscopy. The performance of these nanomaterials in removing pollutants was further assessed by quantifying their adsorption efficiencies towards various organic dyes.[3] The main focus of this research is to clarify how ligand selection affects adsorption capacity, particularly through the interaction between surface-coated QDs and organic pollutants.

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Propagation and Depropagation Kinetics of Tetrahydrofurfuryl Methacrylate Investigated by PLP-SEC

Milena Waldhoff, Philipp Vana

Georg-August University Göttingen, Institute for Physical Chemistry, Göttingen, Germany

Investigating the kinetic behaviour of free radical polymerization systems based on more sustainable resources has been of increasing importance over recent years,[1] thanks to a more environmentally conscious industry and society. In the presented study, propagation rate coefficients k_p, of the high green carbon content monomer, tetrahydrofurfuryl methacrylate (THFMA, k_p^{333K} = 1218 L · mol^{-1}·s^{-1}), are measured by pulsed-laser polymerization (PLP) in combination with size-exclusion chromatography (PLP-SEC).[2] This is done over an extended temperature range (10 °C - 160 °C), allowing the observation of depropagation behaviour as a backwards reaction to propagation. The effective rate coefficient k_p^{eff} can be described through the individual rate coefficients for propagation k_p and depropagation k_{dp} via

$$k_p^{eff} = k_p - \frac{k_{dp}}{[M]} \quad (1)$$

and expresses that the effect of depropagation is inversely proportional to the monomer concentration [M].[3] Arrhenius parameters for forward and backwards directions of the reversible propagation reaction are determined for bulk ($E_{A,p}$ = (20.5 ± 0.7) kJ · mol^{-1}; ln(A_p/L · mol^{-1}·s^{-1}) = 14.11±0.22) and different concentrations of monomer in dimethyl sulfoxide (DMSO) solution. Additionally, another bio-based monomer lauryl methacrylate (LMA, $E_{A,p}$ = (22.3 ± 0.4) kJ · mol^{-1}; ln(A_p/L · mol^{-1}·s^{-1}) = 14.95 ± 0.14, $E_{A,dp}$ = (91.2 ± x9.1) kJ · mol^{-1}; ln(A_p/L · mol^{-1}·s^{-1}) = 34.44 ± 2.42) was investigated in bulk as control system. In extension to the experiments, kinetic simulations performed via PREDICI accurately reproduce the molecular weight distributions (MWD) of the experiments and can also be used to predict kinetic behaviour for different experimental conditions.

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Simultaneous Pressure-Temperature Dependent Luminescence Response of the Eu^{3+}-Activated $BaGeO_3$

Tamilarasu Ganeshamurthy,[1] Christian Hernández-Álvarez,[2] Przemysław Woźny[1], Marcin Runowski [1],

[1]Adam Mickiewicz University, Faculty of Chemistry, Poznan, Poland
[2] Universidad de La Laguna, Departamento de Física, Santa Cruz de Tenerife, Spain

Research on advanced luminescent optical materials is crucial for technology development.[1,2] Simultaneous monitoring of pressure (P)and temperature (T) using luminescent materials is often hindered by the coupling of thermodynamic effects, where the peak shift induced by pressure is also modulated by temperature. This phenomenon causes conventional independent calibration strategies inaccurate, particularly in non-isobaric experimental setups with varied temperature in Diamond Anvil Cells (DACs).[3] This study demonstrates an analytical approach to resolve these problems using $BaGeO_3:Eu^{3+}$ as a model sensor by implementing a 3D analysis of emission spectra collected in a DAC under varying temperature (93-623K) and pressure (up to ≈14 GPa).

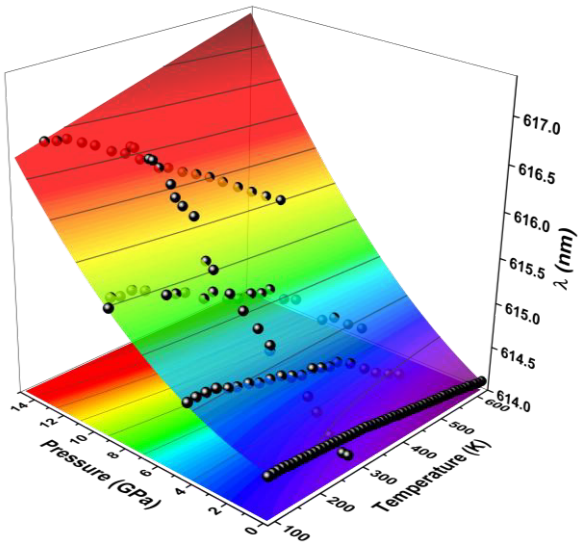

Figure 1:3D surface plot of the Poly2D fit, illustrating the combined effects of temperature and pressure.

Utilizing a second-order polynomial 2D surface fit to model the non-isobaric and non-isothermal data cloud have successfully decoupled the simultaneous physical contributions and quantifies the interaction term F(T.P) the resulting calibration model achieves high predictive accuracy (R^2=0.99), demonstrating a practical methodology to correct for thermodynamic coupling and ensuring reliable dual-mode sensing in extreme environments.

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Covalent polymeric composite materials for gas separation membranes

Daniel Kösters,[1] Philipp Vana[1]

[1] *Institute of Physical Chemistry, Georg-August-University Göttingen, Germany*

Covalent combination of functional materials allows more direct control over the behavior of the resulting composite. This paves the way for complex gas separation membrane materials incorporating multiple specialized functionalities, while reducing compatibility issues.

Covalently linking otherwise incompatible polymers in block copolymeric structures leads to microphase separation and generates well defined morphologies on the nano scale.[1] Upon membrane formation, this microphase separation can have a significant effect on the gas permeability and selectivity of the composite material.[2,3]

One part of this work aims to combine known solution-selective polymeric materials (e.g. 4,4'-(Hexafluoropropylidene)-diphtalic anhydride (6FDA) based polyimides) with highly diffusive 'gutter' polymers (e.g. poly(dimethylsiloxane) (PDMS) or poly(ethyleneglycol) (PEG)) in densely packed bottlebrush block copolymeric architectures.

Due to their high porosity and chemical versatility, metal-organic-frameworks are a promising gas separation membrane material. A key drawback is the low compatibility with the polymer matrix, resulting in difficult membrane formation.[4]

The second part of this work seeks to covalently graft MOFs with known polymeric gas separation materials, in order to combine the advantageous properties of both techniques in mixed-matrix-membranes (MMMs). In a first step, UiO-66-NH2 MOFs are grafted with individual homopolymers (e.g. polyimide and bottlebrush-PEG), to assess functionalization rate, compatibility and performance. Subsequently, highly functional materials from part one of this work will be combined with the MOFs to achieve complex composite membranes.

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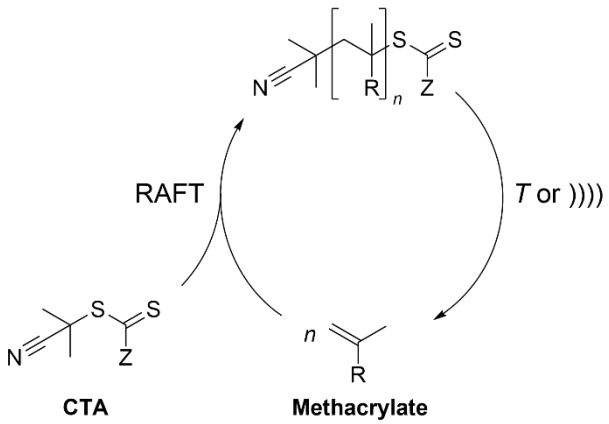
Radical Depolymerization Under Aspects of Sustainability

Samuel Che Jonah Wendler, Philipp Vana

Georg-August University Göttingen, Institute for Physical Chemistry, Göttingen, Germany

In the context of subsequent recycling strategies and focusing on principles of green chemistry, the depolymerization of biobased polymethacrylates under thermal and ultrasonic conditions is explored. For that, methacrylates are polymerized in a controlled radical mechanism, using RAFT (Reversible Addition–Fragmentation chain-Transfer) polymerization and partially renewable resources. The chain-transfer agent (CTA) of the RAFT polymerization is utilized as end-group with a weak C–S bond, allowing a homolytic bond breakage as initial step for a subsequent depolymerization and monomer recovery.



Scheme 1: CTA-mediated RAFT polymerization and subsequent depolymerization.

To reverse polymerization, high temperatures are needed, typically over 300 °C, but decreasing the concentration decreases also the necessary temperature. The thermal approach at 120 °C can successfully extrapolate the literature[1] known monomer recovery for new biobased polymethacrylates, achieving an impressive recovery of 89 % after 1 hour for tetrahydrofurfuryl methacrylate without any additional initiator being present.

A polymer degradation is also observed under ultrasonic irradiation but usually due to a bisection near the centre of the chain.[2] In contrast, it is investigated if a targeted activation of the C–S bond of CTA-functionalized chain ends is possible to initiate monomer recovery, using the CTA as sono-iniferter.[3,2] Additionally, a chain end-functionalization of unfunctionalized polymer for subsequent thermal depolymerization is aimed for.

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Dimerization Reactions of of Aryl-Substituted Bicyclobutanes (BCBs) under Acid-promoted Conditions

Daniil A. Knyazev,[1,‡] Malini George,[1,‡] Kamil Swiatek[1] and Daniel B. Werz[1,*]

[1]*Albert-Ludwigs-Universität Freiburg, Institute of Organic Chemistry, Albertstr. 21, 79104 Freiburg (Germany)*

Email: daniel.werz@chemie.uni-freiburg.de

‡ *These two authors contributed equally.*

Bicyclo[1.1.0]butanes (BCBs) have emerged as rigid three-dimensional bioisosteres of aromatic systems, supporting the "escape from flatland" concept in medicinal and agrochemical chemistry.[1] Owing to their exceptionally high ring strain, BCBs are far more reactive than donor–acceptor cyclopropanes and readily undergo strain-release transformations under Lewis or Brønsted acid or photochemical activation.[2] These reactions are typically dominated by 1,3-difunctionalization pathways, but unusual nucleophilic behavior of the central bond often leads to cyclobutene by-products.[3] Prompted by these side reactions, we examined the self-reactivity of BCBs under acidic conditions. This study revealed a previously unrecognized dimerization pathway featuring an unprecedented 1,3-dipolar reactivity involving the aryl substituent.

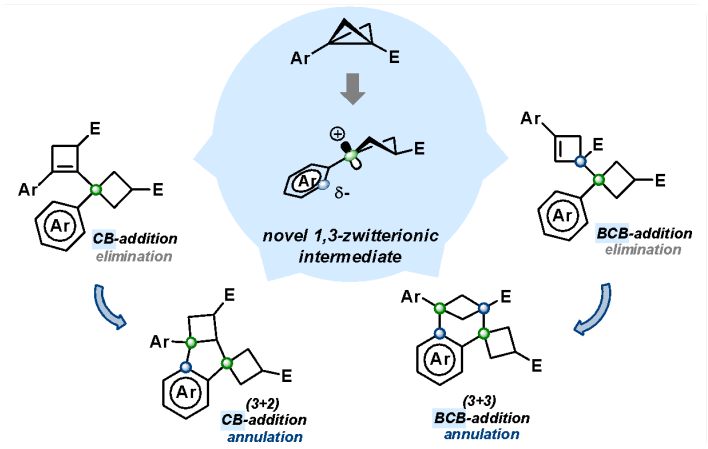

Figure 1: Major BCB dimerization pathways

Depending on the pathway, the reaction furnishes a variety of different dimers, especially we highlight a spiro-annulated indane scaffold or a spirotetrahydronaphthalene bearing a bridging methylene unit. Mechanistic studies explain the origin of this divergent reactivity. These findings are of fundamental relevance for BCB chemistry, as such dimerization can act as a competing background process in Lewis or Brønsted acid-catalyzed reactions, potentially lowering yields.

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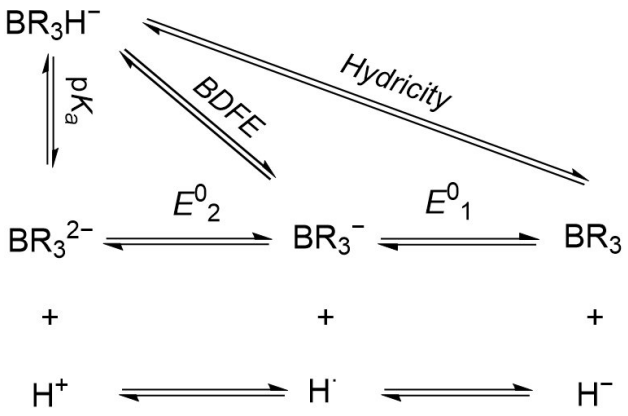
Redox Reactivity of Triarylboranes

Sophie Dequiedt[a], Frederick Giebelhausen[a], Hanna Graf[a], Lewis Hess[a], Amelie Rein[a], Felix Meyer[a], Inke Siewert[a]

[a]*University of Göttingen, Institute of Inorganic Chemistry, Göttingen Germany*

Borohydrides are ubiquitous stoichiometric hydride donor reagents for the reduction of carbonyl compounds, however their synthesis and use are associated with high energy demand and a lot of waste. The crucial parameter quantifying the hydride transfer reactivity is the thermodynamic hydricity ($\Delta G^0_{H^-}$), which denotes the ability to donate a hydride ion of a given species.[1] The hydricity can be derived by the free energy of proton and electron transfer steps.[2] In other words, it is linked to the bond dissociation free energy (BDFE) and first reduction potential (see Eq. 1 and Scheme 1). Borohydrides span a large range of hydricities ranging from 0.6 to 159.22 kcal mol^{-1} in MeCN exemplifying their tunabilty.[3]

$$\Delta G^0_{H^-} = 2.303RT\mathrm{p}K_a + zFE^0_2 + \Delta G^0_{H^+|H^\cdot} + zFE^0_1 + \Delta G^0_{H^\cdot|H^-} \quad (1)$$



Scheme 1: Schematic relationship between the Hydricity and Redoxpotentials [3]

Within our project we target the formation of borohydrides by electrons and protons starting from the borane. Crucial for this approach is the stability of the radical species BR_3^- and the redox potential of the borane BR_3.
We synthesized and investigated the electrochemical properties of Aryl-boranes with different charged groups to tune their redox properties. Arylboranes were used due to their enhanced stability of the radical anion, which was investigated by CV. The results of this investigation will be presented.

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Cooperative Asymmetric Catalysis Under Confinement

A. Bauer[1], Dr. E. Goldstein[2], Dr. M. Nandeshwar[2], L. Rautenbach[1], Prof. Dr. M. R. Buchmeiser[2], Prof. Dr. R. Peters[1]

[1] *Universität Stuttgart, Institute für Organische Chemie, Pfaffenwaldring 55, 70569 Stuttgart Germany*

[2] *Universität Stuttgart, Institute für Polymerchemie, Pfaffenwaldring 55, 70569 Stuttgart Germany*

Our research group has developed numerous homogenous polyfunctional catalysts.[1-2] The design was inspired by enzymes with various functional groups of a catalyst system work in concert to accelerate and control a chemical reaction. This enables the simultaneous activation of the substrates and high catalytic activity and stereo control to be achieved. Based on this performance cooperative Catalyst should be investigated in heterogeneous catalysis to analyse its behaviour under confinement in mesoporous materials. In order to respond to the primary question, whether the entropic advantage of enzymes can be transferred to artificial immobilized bifunctional catalysts through confinement effects? This work presents the successful synthesis of a trimethoxysilyl linker-modified cooperative catalyst and the results of the heterogeneous studies.

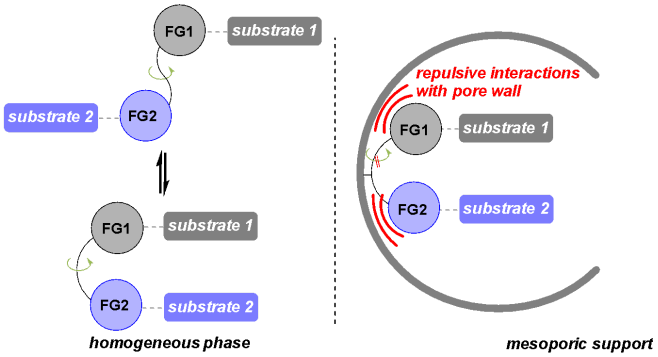

Figure 1: Rigidified catalyst under confinement

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Working Under Pressure: Empirical Findings on the Challenges Facing PhD Students in Chemistry

Alexandra Tietze[1], Anna Röhnelt[1], Laura Hillebrand[1], Sylvia Schlöglmann[1], Monja Schilling[1], Chris M. Wanner[1], Katrin Beuthert[1]

[1] *Gesellschaft Deutscher Chemiker e.V., Frankfurt am Main, Germany*

This study presents results from a nationwide survey of PhD students in chemistry and related disciplines in Germany. The data reveals considerable challenges across all domains of the survey: 61% had considered discontinuing their PhD, citing mental health issues, poor supervision, and high workloads (Fig. 1). Satisfaction with supervision correlated strongly with feedback quality, leadership, and communication skills ($r = .72–.78$, $p < .001$). Over half reported working more than 45 hours per week, and one fifth could not cover living expenses with their income. Reports of discrimination, power abuse, and inadequate career support further highlight systemic shortcomings. The findings point to a need for comprehensive reforms in PhD education, including clearer supervision structures, sustainable funding, and institutional mechanisms to support well-being and career development. Improving the PhD phase is not only a matter of fairness but also vital to preventing talent loss and ensuring the long-term sustainability of academic research.

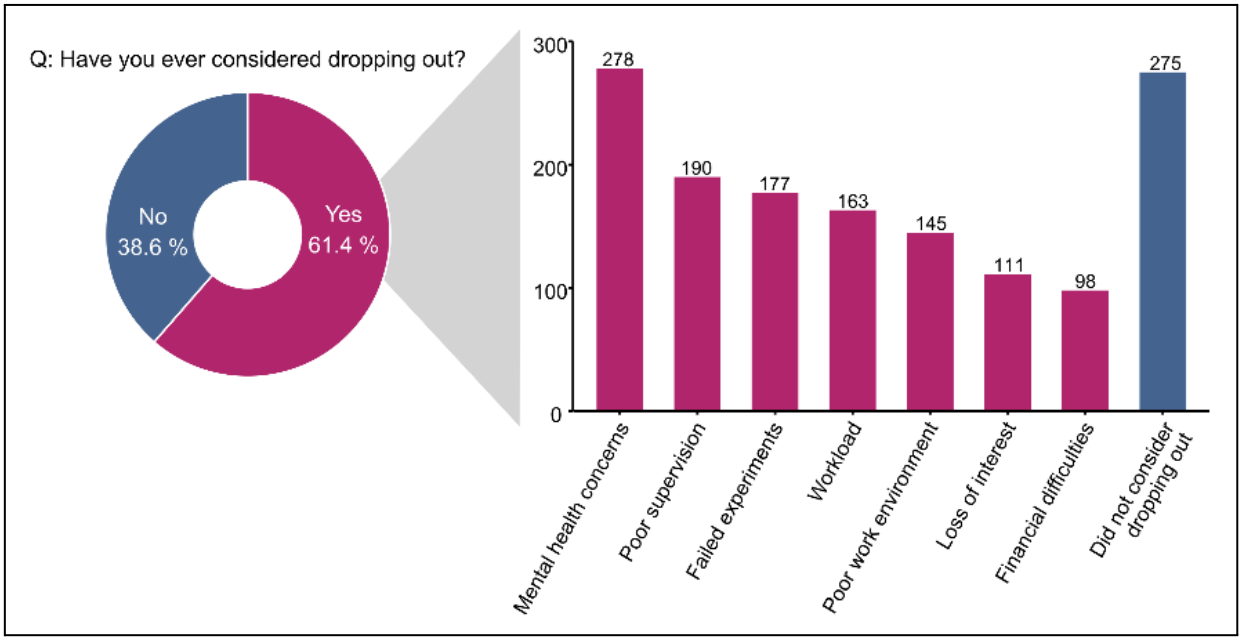

Figure 1: Consideration of dropping out. Multiple answers possible, n = 722.

Effect of Natural Zeolite (Clinoptilolite) on Heavy Metal Content in Lemon Balm (*Melissa officinalis* L.)

Snežana Tošić,[1] Denis Mitov,[1] Jelena Mrmošanin,[1] Stefan Petrović,[1] Katarina Milenković,[1] Aleksandra Pavlović,[1]

[1] *University of Niš, Faculty of Sciences and Mathematics, Niš, Serbia*

Soil pollution with heavy metals represents one of the most significant environmental problems today. Plants growing on contaminated soil can uptake heavy metals and thus pose a health risk to humans who consume them. To reduce the uptake of heavy metals, various techniques can be applied, such as the addition of biochar, bentonite, or zeolite.[1,2] In this study, the effect of adding the natural zeolite clinoptilolite to soil artificially contaminated with Cd on the pseudototal contents of Cd, Co, Cu, Fe, Mn, and Zn in lemon balm (*Melissa officinalis* L.), as well as on the concentrations of bioavailable elements in the soil, was investigated through a pot experiment. The soil was doped with Cd at a concentration of 20 mg/kg, and zeolite was added to three pots at rates of 5, 10, and 20 g/kg of soil, after which one-month-old lemon balm seedlings were planted. After 75 days, the plants were harvested, the roots were separated from the aboveground parts, and soil samples were collected for analysis.

Soil and plant samples were prepared for analysis by microwave digestion, while the amounts of bioavailable elements in the soil were determined by extraction with a DTPA solution.[3] The prepared samples were analyzed using ICP-OES with a method of external calibration curve. The application of zeolite at rates of 5, 10, and 20 g/kg reduced the concentration of bioavailable Cd by 16.5%, 29.8%, and 13.5%, respectively, compared to the treatment without zeolite. The application of zeolite also reduced the bioavailable concentrations of all other determined elements. Zeolite application led to a reduction in the contents of the determined elements in the roots (with the exception of Cu and Zn at zeolite application rates of 10 and 20 g/kg) and of Cd in the shoots of lemon balm (from 4.22 ± 0.01 mg/kg in the treatment without zeolite to 2.67 ± 0.02 mg/kg with the application of 20 g/kg zeolite). The contents of the other analyzed elements in the shoots of lemon balm did not change significantly with zeolite application.

Based on the results obtained, it can be concluded that the application of zeolite positively affects the reduction of bioavailable concentrations of Cd, Co, Cu, Fe, Mn, and Zn in soil and can also lead to reduced Cd uptake by lemon balm, thereby improving its safety for use for medicinal purposes.

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Effect of thermal processing on polyphenol content, flavonoids, and antioxidant activity of *Rosa dumalis* Bech. fruits

Aleksandra Pavlović,[1] Katarina Milenković,[1] Jelena Mrmošanin,[1] Denis Mitov,[1] Stefan Petrović,[1] Milena Nikolić,[2] Snežana Tošić[1]

[1] *University of Niš, Faculty of Sciences and Mathematics, Department of Chemistry, Niš, Serbia*

[2] *Academy of Professional Studies South Serbia, Department of Technology and Art, Leskovac, Serbia*

Wild rose fruits are well known as a rich source of bioactive compounds with pronounced antioxidant properties; however, thermal processing may lead to their degradation. The aim of this study was to investigate the effect of cooking temperature on the total polyphenol and flavonoid content, as well as on changes in the antioxidant activity of *Rosa dumalis* Bech. fruits.

The samples were subjected to cooking at 70, 80, and 90 °C for different time intervals. Total polyphenol and flavonoid contents were determined spectrophotometrically, while antioxidant activity was evaluated using the DPPH assay. The kinetics of thermal degradation were analyzed using a first-order reaction model, and activation energies were calculated from the Arrhenius equation.[1]

The results showed that increasing cooking temperature and time led to a significant decrease in total polyphenol and flavonoid contents, accompanied by a reduction in antioxidant activity. The lowest losses of total polyphenols and flavonoids were observed after 125 minutes of cooking at 70 °C, whereas the highest losses occurred after 125 minutes at 90 °C. The degradation process followed first-order reaction kinetics, with activation energies of 43.9 kJ mol^{-1} for total polyphenols and 56.9 kJ mol^{-1} for total flavonoids. A strong positive correlation ($r > 0.97$) was found between the decrease in these bioactive compounds and antioxidant activity. The results obtained are comparable with literature data.[2]

These findings indicate that temperature plays a crucial role in preserving the bioactive potential of *Rosa dumalis* Bech. fruits during thermal processing and may be important for the optimization of technological processes in the production of food and functional products.[3]

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London Dispersion Stabilized *meta*-Bisazobenzenes – Combining New Concepts for MOST Applications

Inga L. Schneider,[1,2] Kai Hanke,[1,2] Dominic Schatz[1,2], Hermann A. Wegner[1,2]

[1]*Justus-Liebig University, Institute of Organic Chemistry, Giessen, Germany*

[2]*Justus Liebig University, Center of Materials Research (ZfM/LaMa), Giessen, Germany*

Molecular solar thermal (MOST)-systems offer a promising strategy for long-term storage of solar energy in molecules. The energy of light is converted into chemical energy and released as heat with full regeneration of the initial material. These systems consist of molecular pairs that undergo photoisomerization upon irradiation.[1] Azobenzene is one of the most promising MOST-systems. The compound can be switched between its stable (*E*)-isomer as the ground state and the energetically higher, metastable (*Z*)-isomer representing the storage state. When designing new compounds for application in MOST-systems, one focus is on increasing this energy gap and thereby enhancing the energy storage density.[2]

In this study, two factors should improve the energy storage density: Firstly, two decoupled switching units are integrated into one molecule, thereby reducing the relative molecular weight per switching unit while maintaining the storage capacity.[3] Secondly, the presence of alkyl-residues in the *ortho*-position of the outer phenyl units of a *meta*-bisazobenzene are expected to stabilise the (*E*)-isomer *via* London dispersion interactions. This should lower the energy of the ground state, thereby increasing the energy gap between the ground and the storage state and thus resulting in an increased energy storage density. (Figure 1).[4]

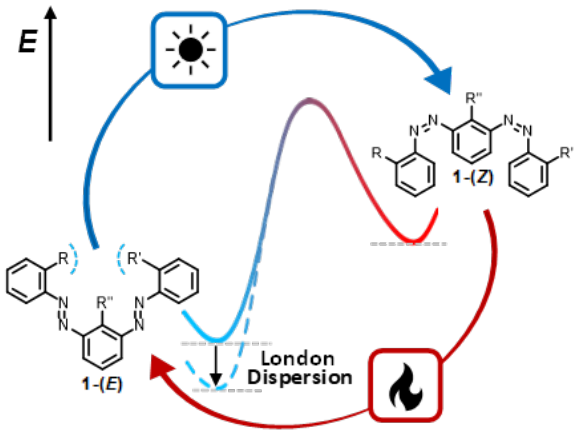

Figure 1: London dispersion stabilized *meta*-bisazobenzene **1** as a MOST-system.

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Characterization of the Initial Lithiation Step in FeS_2 All-Solid-State Lithium-Sulfur Batteries

Sophie Richter,[1] Matilde Pavan,[2] Timo Weintraut,[1] Jürgen Janek,[2] Anja Henss[1]
[1] *Justus Liebig University, Institute for Experimental Physics 1, Giessen, Germany*
[2] *Justus Liebig University, Institute for Physical Chemistry, Giessen, Germany*

All-solid-state lithium-sulfur batteries (ASSLSBs) are promising candidates for the storage of energy due to the low cost and the high energy densities of the used materials. One promising candidate for the active material in positive electrodes is iron disulfide, FeS_2. The latter has a high theoretical capacity (894 $mAh \cdot g^{-1}$), it is naturally abundant and environmentally benign.[1] In contrast to classic positive electrode materials, like lithium nickel manganese cobalt oxide (NMC), which show intercalation reactions, FeS_2 undergoes a conversion reaction. Here, the redox states of the single elements are altered, leading to multiple electron transfers and therefore higher theoretical capacities than *e.g.* NMC.

The reactions during cycling of the FeS_2 ASSLSB are still under investigation (a suggested mechanism is displayed in Fig. 1). In this work we focus on the initial lithiation reaction of the material and employ secondary ion mass spectrometry (SIMS) and x-ray photoelectron spectroscopy (XPS), together with electrochemical measurements, to ascertain how the depth of discharge at the initial lithiation of the material influences the degradation and the lifetime of the cell.

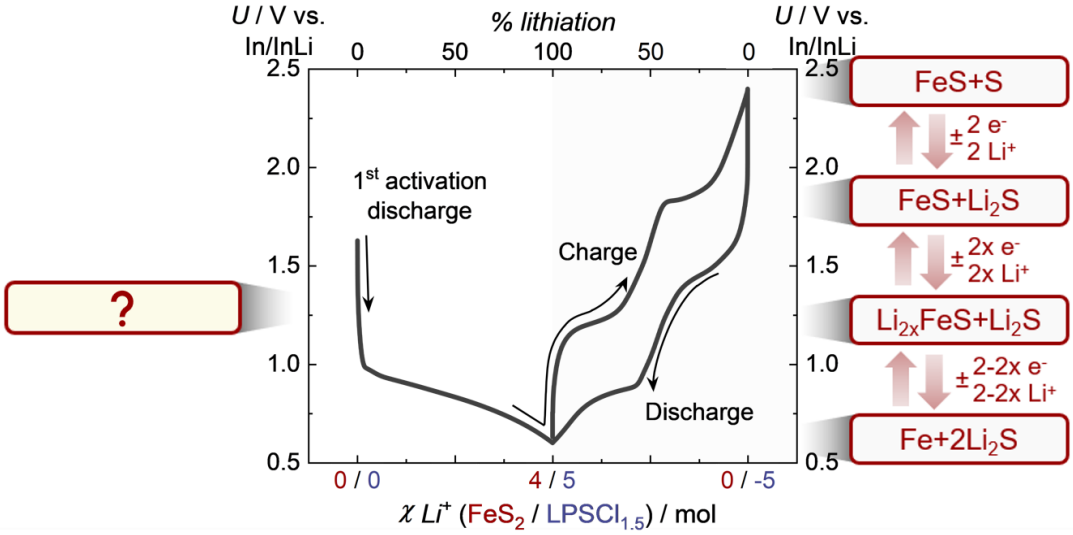

Figure 1: Proposed reaction mechanism of FeS_2 in ASSLSBs during the initial lithiation and cycling. The figure is adapted from Pavan *et al.*[2]

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Efficient Prediction of Singlet-Triplet Gaps at DFT Accuracy Using the g-xTB Method

Benedikt Bädorf,[1] Thomas Froitzheim,[1] Andreas Hansen,[1] Jorge Campos-Gonzales-Angulo,[2] Alán Aspuru-Guzik,[2] Stefan Grimme[1]

[1] *University of Bonn, Mulliken Centre for Theoretical Chemistry, Bonn, Germany*
[2] *University of Toronto, Department of Computer Science, Toronto, Canada*

Finding emitters that are more energy-efficient and are degradation stable in organic light-emitting diodes (OLEDs) is of great interest in display-technology research. A crucial property of such emitters is a small singlet–triplet (S–T) gap, which enables the conversion of “dark” triplet states into “bright” singlet states, as realized in state-of-the-art thermally activated delayed fluorescence (TADF) emitters.[1]

We demonstrate that the new g-xTB[2] quantum chemistry method can compute S–T gaps with an accuracy approaching that of density functional theory (DFT), while reducing computational cost by nearly two orders of magnitude. The calculated gaps are benchmarked against high-level theoretical and experimental data, highlighting the robustness of g-xTB. Even the potentially emerging new class of emitters with inverted single-triplet gaps (INVEST) can be computed accurately by the method.[3]

This capability, for example, enables a drastic improvement in screening approaches for novel emitter molecules,[4] for which we provide practical guidelines.

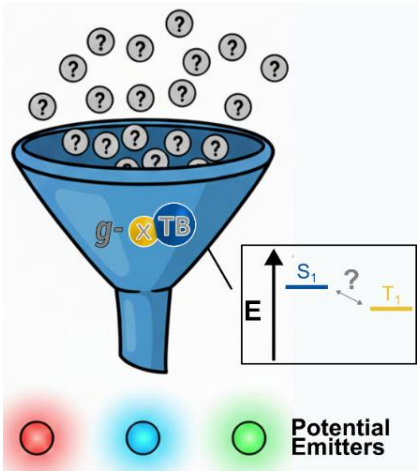

Figure 1: Schematic depiction for the application of g-xTB in the screening of S-T gaps

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Tuning of Arsenic Corrole Complexes by Axial Coordination: From Photophysics to Photosensitization

Marla Brandstäter,[1] Hendrik Peters,[2] Anastasiia Riabchunova,[1] Michael Karnahl,[1] Martin Bröring,[2] Stefanie Tschierlei[1]

[1] *TU Braunschweig, Institute for Physical and Theoretical Chemistry, Braunschweig, Germany*
[2] *TU Braunschweig, Institute of Inorganic and Analytical Chemistry, Braunschweig, Germany*

Corroles, contracted porphyrin analogues, exhibit unique redox and excited-state characteristics.[1,2] Although they show promise as photosensitizers, arsenic corroles remain largely uninvestigated.[3] In this study, we introduce a series of arsenic corroles bearing systematically varied axial ligands to probe how axial coordination modulates their photophysical properties and function.[4]

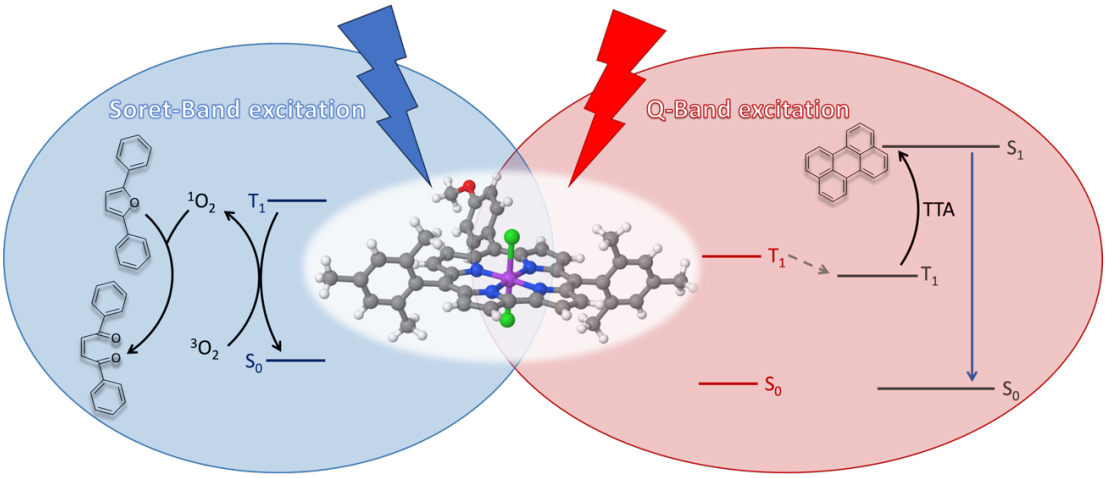

Figure 1: Applications of arsenic corroles via the excited triplet state with Soret- and Q-Band excitation

Using steady-state absorption and fluorescence, time-resolved emission spectroscopy, and nanosecond transient absorption, we construct a comprehensive excited-state landscape and demonstrate efficient population of long-lived triplet states. By comparing different oxidation states and donor versus acceptor axial ligands, we uncover clear structure-property relationships that directly influence photosensitizer performance. Direct detection of singlet oxygen ($^1O_2$) confirms robust photosensitization, and the photooxidation of 2,5-diphenylfuran (DPF) to DBE illustrates a practical application. Under continuous irradiation, photostability is found to depend strongly on the nature of the axial ligand.[4] Finally, low-temperature spectroscopy and triplet–triplet annihilation upconversion experiments offer mechanistic insights and inform ligand design. Overall, axial coordination emerges as a straightforward strategy to tune both activity and stability, positioning arsenic corroles as versatile, customizable photosensitizers.

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JCF Team Mentale Gesundheit

Alena Neudert, Emilia Wilkesmann, Laura Hillebrand, Felicitas von Usslar, Alexandra Tietze, Tom Götze-Ebert, Felix Zhu, Jana Maria Grüneberg, Irene Boeck

Das Team Mentale Gesundheit ist eines der Teams vom JCF (JungesChemieForum). Ziel des Teams ist es, die Aufmerksamkeit und Sichtbarkeit von mentaler Gesundheit zu erhöhen und entsprechende Hilfsangebote bereitzustellen. In diesem Zusammenhang wurde beispielsweise eine Übersicht von Beratungsstellen erstellt, die nach Bundesland und Universität geordnet ist. Eine weitere Möglichkeit bietet das Mentoring-Programm, welches dieses Jahr nach zwei erfolgreichen Durchgängen in die dritte Runde startet. Das JCF-Mentoring-Programm stellt jüngeren Studierenden Mentor:innen aus dem Masterstudium oder der Promotion zur Seite. Im Programm geht es darum, Erfahrungswissen weiterzugeben, den Blickwinkel auf Probleme für die Mentees zu verändern und den Support und die Kommunikation zwischen Studierenden und Promovierenden zu stärken. Neben vielen Workshops und Vorträgen zu Themen wie dem Imposter-Syndrom, Burnout, Uncertainty in a PhD, Achtsamkeit und Mental Health First Aid gibt es außerdem noch anonyme Erfahrungsberichte aus der wissenschaftlichen Community auf der Team-Website zu finden, in denen die Autor:innen frei über ihre Probleme im Studium oder der Promotion berichten können. Neu dazugekommen und im GDCh-Shop erhältlich ist der Selfcare-Pass. Dieser ist ein Online-Wegweiser für mentale Gesundheit und ebenfalls auf der Team-Website zu finden.[1] Der Pass besteht aus einfachen Übungen, Impulsen und Reflexionshilfen, die helfen können, mehr Achtsamkeit, Balance und Selbstfürsorge in den Alltag zu bringen.



Figure 1: Selfcare-Pass und Mentoringprogramm Mental Mentor

References:

[1] https://jcf.io/teams/mentale-gesundheit

Shape Memory Polyurethane Foams: Innovative Solutions for Safer and Sustainable Applications.

Anna-Lisa Poser[1,2]

[1] *Fraunhofer Institute for Applied Polymer Research IAP, Department of Shape Memory Polymers, Potsdam, Germany*

[2] *University of Potsdam, Institute of Chemistry, Potsdam, Germany*

Polyurethane (PU) foams are extensively used in modern society, appearing in products such as upholstery, insulation, and various everyday items. However, their large volume can be problematic, as significant space is required during transportation and storage. Producing PU foam on-site is an alternative, but it involves handling isocyanates, which pose serious occupational health and safety risks, including respiratory irritation and long-term health effects.[1] Shape memory polymers (SMPs) present an innovative solution to these issues. As “smart materials”, SMPs change shape in response to external stimuli such as temperature.[2] This is achieved through a thermomechanical “programming step”: 1) heating above the phase-transition temperature, 2) loading, 3) cooling below the phase-transition temperature, and 4) unloading. Upon heating, the material then returns from the “programmed shape” to its original form (one-way shape memory effect), while some SMPs perform reversible actuation between two semi-stable states (two-way shape memory effect (2W SME)).[3] Our group implemented both effects into PU foams for innovative building applications. Programmed PU foam may exhibit a 2W SME with a maximum actuation of 22.7 %. Such behaviour could reduce energy consumption by up to 45 % in certain scenarios (Fig. 1A).[4] In 2025, the concept of FOIM (FOIl + foaM) was introduced. The material can be compressed into a translucent foil and recovers shape upon heating to 45 °C, thus exhibiting a recovery ratio of 99.5 % and an increase in height increase by 1600 % (Fig. 1B).[5]

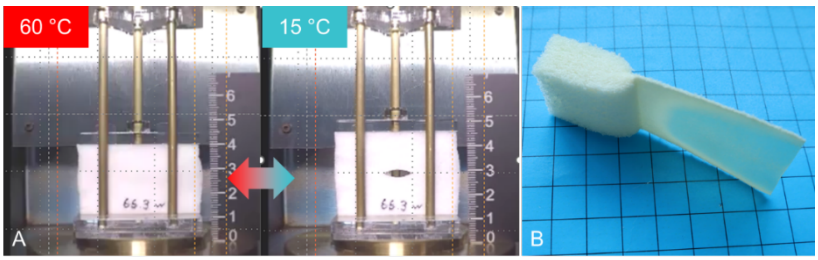

Figure 1: Depiction of the A. actuating foam[4] and B. of the FOIM[5].

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Novel Azaborine-Based Inhibitors of Histone Deacetylases (HDACs)

Martin Behringer, Markus Schweipert, Enna E. Peters, Aleksandra Kopranovic and Franz-Josef Meyer-Almes

Department of Chemical Engineering and Biotechnology,
University of Applied Sciences Darmstadt, 64295 Darmstadt, Germany

Aromatic ring systems are widely found in biologically active pharmaceutical compounds, including FDA-approved histone deacetylase inhibitors (HDACs).[1] These enzymes are implicated in a wide range of diseases, including cancer, neurodegenerative disorders, inflammatory and autoimmune diseases, and metabolic disorders.[2] However, the presence of aromatic systems often leads to reduced aqueous solubility of the inhibitors, which can limit therapeutic applicability. One approach to overcoming this limitation is the replacement of conventional aromatic rings with azaborine moieties, formed by substituting two adjacent carbon atoms with boron and nitrogen.[3] The incorporation of B–N analogues not only expand structural diversity but also offers a means to circumvent existing patent-protected scaffolds. In this work, azaborines isosteric to naphthalene and indole were synthesized and employed as capping groups in the design of HDAC inhibitors. These compounds were conjugated to a range of aliphatic and aromatic linkers bearing different zinc-binding groups derived from known active molecules. Of the twenty-four compounds evaluated, nearly half showed inhibitory activity against at least one of the enzymes HDAC1, HDAC4, or HDAC8, with three exhibiting nanomolar IC_{50} values (Figure 1).[4] These results demonstrate that azaborine building blocks can be successfully incorporated into HDAC inhibitors without compromising activity, thereby indicating the potential of azaborine-containing scaffolds for the development of active compounds targeting other biological systems.

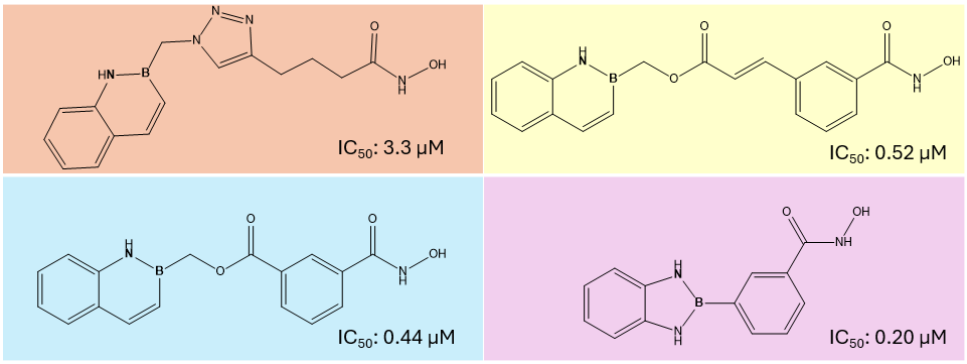

Figure 2: Selection of azaborine-based inhibitors with their IC_{50} values against HDAC8.

References:

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Advancing Dispersion Corrections in Computational Chemistry

Marvin Friede,[1] Thomas Froitzheim,[1] Stefan Grimme[1]

[1] *University of Bonn, Mulliken Center for Theoretical Chemistry, Bonn, Germany*

Despite being the individually weakest non-covalent interaction, London dispersion forces are critical for understanding the behaviur of complex chemical and biological systems. These forces are ubiquitous (even for neutral and non-polar systems), always attractive, and grow with increasing system size, making them essential for everything from protein folding to catalyst design.[1,2]

In this work, we examine the treatment of dispersion within computational chemistry, focusing on the widely used DFT-D*n* (*n*=1-4) series.[3,4] These semi-classical corrections follow the fundamental London formula:

$$E_{disp} = -C_6 R^{-6} \quad (1)$$

We discuss the evolution of these methods, showing how each generation increased sophistication – moving from fixed, empirical parameters to *ab initio*, environment-dependent dispersion coefficients (C_6). While this evolution significantly improved accuracy, the DFT-D methods retain the computational efficiency required for large systems. Myriad (density functional theory) benchmarks show that adding a dispersion correction not only dramatically improves the accuracy for non-covalently bound systems but also for thermochemistry and reaction barriers.[5]

Finally, we present ongoing developments towards the next-generation dispersion correction (DFT-D5). This new iteration aims for higher accuracy, an improved treatment of charged systems, and additional robustness for uncommon coordination patterns.

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Turning lignocellulosic biomass into sustainable polymer materials

Alice Cappitti, [1] Antonella Salvini [1]

[1] *Department of Chemistry "Ugo Schiff", University of Florence, 50019 Sesto Fiorentino, Italy*

In recent years, increasing awareness of the economic and environmental drawbacks associated with fossil resource exploitation has driven the search for more sustainable and eco-friendly alternatives. In this context, lignocellulosic materials, particularly those derived from waste streams or industrial by-products, have emerged as promising renewable resources for the development of high-value biopolymers and advanced materials, thanks to their biodegradability, renewability, recyclability, and widespread availability.

This study explores different strategies for the valorization of lignocellulosic biomass aimed at developing innovative materials for a wide range of applications. One approach exploits lignocellulosic feedstocks for the synthesis of bio-derived monomers and their corresponding biopolymers. In particular, saccharide-derived biomonomers, characterized by polar and reactive functional groups, enable the development of acrylic and vinyl copolymers with tunable properties, enhancing material performance while improving sustainability and recyclability. Applicative testing confirms their potential in advanced adhesive systems and other polymer formulations [1]. In parallel, bio-based materials such as composite panels and cellulose-based films are produced through tailored biorefinery protocols, including specific pre-treatment processes and solubilization of the cellulose fraction from natural or waste fibers, enabling the comprehensive valorization of lignocellulosic biomass and further expanding opportunities for sustainable material design.

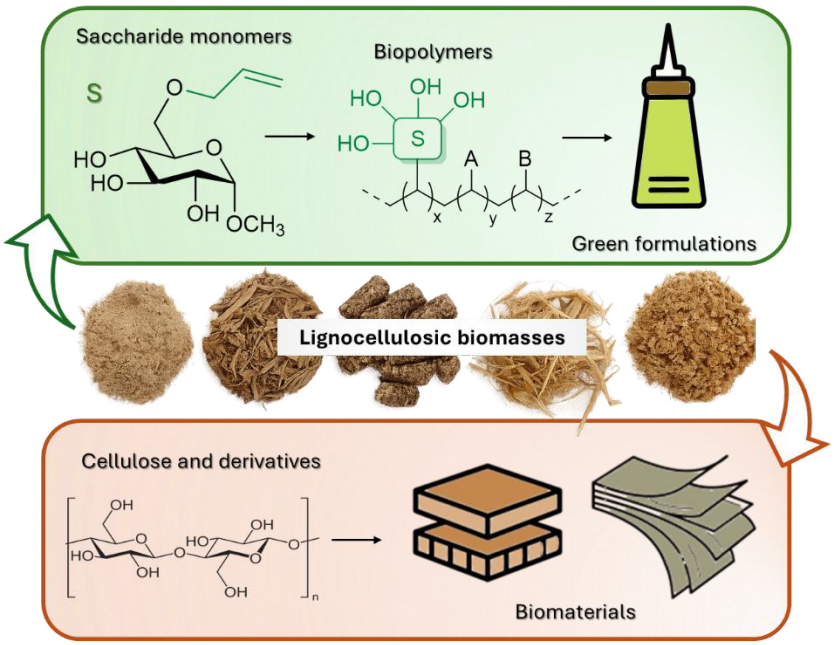

Figure 1: from lignocellulosic biomass to *green* formulations and biomaterials

References:

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P52

Mechanochemical Control of the Dehydration Degree of $CuSO4 \cdot 5H_2O$ by Vessel Material

Steffi Krause Hinojosa,[1] Prof. Dr. Lars Borchardt[1]

[1] *Ruhr Universität Bochum, Inorganic Chemistry I, Germany*

Selective control over the degree of hydration in crystals remains a significant challenge in solid-state chemistry, as dehydration typically proceeds uncontrollably through multiple hydrate phases upon thermal activation. Mechanochemistry offers an alternative activation mode, where mechanical energy directly conducts solid-state transformations, yet its potential for controlling dehydration pathways remains largely unexplored. Here, we demonstrate that mechanical energy alone is sufficient to induce and control the dehydration phase of copper(II) sulfate pentahydrate ($CuSO_4 \cdot 5H_2O$)[1], enabling selective access to defined hydration states under solvent-free conditions. Milling experiments were performed at 30 Hz for 90 minutes show that the degree of dehydration is driven by mechanochemical parameters rather than temperature, with the milling vessel material acting as a crucial modulator of the process. Using polymer vessels with distinct surface properties, namely polymethyl methacrylate (PMMA) and perfluoroalkoxy alkane (PFA), under identical conditions, notable phase selectivity is observed (see **Figure 1**). Milling in hydrophilic PMMA vessel predominantly results in the formation of trihydrate phase ($CuSO_4 \cdot 3H_2O$), whereas milling in hydrophobic PFA promotes deeper dehydration, yielding the monohydrate phase ($CuSO_4 \cdot H_2O$), as confirmed by PXRD and Raman spectroscopy. We propose that the vessel material influences the mechanochemical dehydration by regulating the effective water activity within closed milling system. While hydrophilic PMMA vessel temporarily retains mechanically released water, stabilizing intermediate hydrate phases, hydrophobic PFA suppresses water adsorption and facilitates further dehydration. These results establish mechanochemistry as a powerful method to control dehydration reactions through mechanical energy and highlight vessel material as a critical parameter in solid-state chemistry.

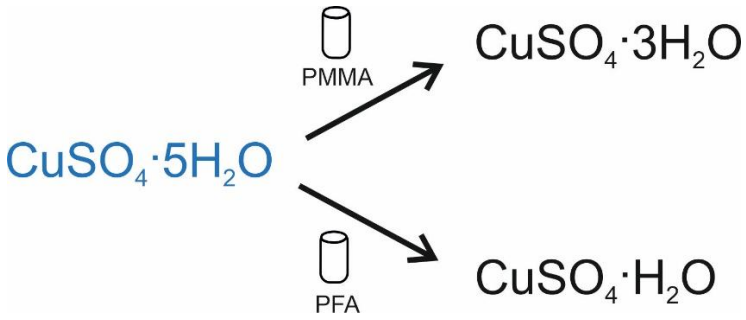

Figure 1: Reaction scheme for the mechanochemical dehydration of $CuSO_4 \cdot 5H_2O$ in PMMA and PFA vessels.

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Selective Boost of Spin Diffusion Pathways under Site-Specific DNP

E. R. Bensons,[1] T. Biedenbänder,[1] J. Klütz,[1] B. Corzilius[1,2]

[1] *University of Rostock, Institute of Chemistry and Department LLM, Rostock, Germany*

[2] *Leibniz Institute for Catalysis, Rostock, Germany*

Magic-angle spinning (MAS) solid-state NMR is a unique technique in the repertoire of analytical methods for structural biology and materials science. In the past decade its application has undergone significant advancements through the development and commercialization of dynamic nuclear polarization (DNP) which significantly increases sensitivity, allowing for previously deemed unfeasible experiments. DNP utilizes the polarization transfer from free electrons to nuclei during microwave irradiation of the electron resonances yielding a significant hyperpolarization of the sample.

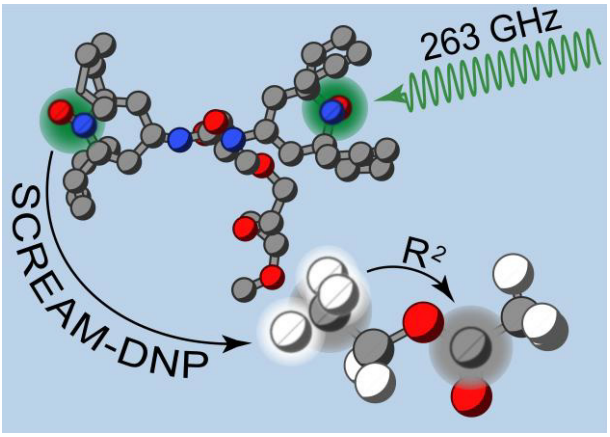

Figure 1: Stylized polarization transfer from the electron source (biradical AMUPol) to the ethyl acetate model compound.

A significant interest in the field lies in the investigation of the processes that occur during the DNP experiment, both to enhance comprehension and to leverage this knowledge to develop DNP-exclusive experiments. In this work the light is shed on the ^{1}H-^{13}C cross relaxation process that is active in methyl groups at 100 K and is used to site-specifically introduce hyperpolarization. Once polarization is transferred to methyl carbons it further spreads through ^{13}C-^{13}C spin diffusion to carbon atoms in proximity. This serial process is exclusively active under DNP and is utilized in the SCREAM-DNP (Specific Cross-Relaxation Enhancement by Active Motions under DNP) experiment.[1] The central objective of this work is the optimization and utilization of the spin diffusion process that spreads the polarization from the methyl groups through the ^{13}C network. A key question here is the MAS dependence of the rate constant which we investigated in an ethyl acetate model compound. We successfully confirmed our hypothesis that the spin diffusion rate constant is strongly MAS-dependent and experiences a significant increase with the recoupling conditions of rotational resonance. These findings demonstrate that the reintroduction of the dipolar coupling can also be used for the selective boost of polarization transfer pathways.[2] In summary this work focuses on the fundamental investigation of the processes active under DNP but also with the goal in mind to use this knowledge for further improving the methodological portfolio of DNP.

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Low dimensional perovskites in metal halide perovskite solar cells

Malwine Lühder[1,2], Lukas Wagner[1,2], Jan Christoph Goldschmidt[1,2]

[1] *Marburg University, Physics of Solar Energy Conversion Group, Marburg, Germany*

[2] *mar.quest | Marburg Center for Quantum Materials and Sustainable Technologies*

Low dimensional perovskites (LDPs) are currently being investigated as surface passivation and charge blocking layers for stable perovskite solar cells, a cheaper and less resource consuming[1] alternative to silicon-based solar cells. LDPs exhibit excellent opto-electronic properties like a tunable band gap[2] and effectively reduce the recombination rate of electron-hole pairs at layer interfaces in the solar cell stack.[3] The hydrophobic nature of the alternating organic cation layers prevents moisture-induced degradation of the 3D bulk perovskite and enhances the long-term stability of the device.[4] Figure 1 schematically depicts how the introduction of LDPs can help to overcomes the main challenges of perovskite solar cells.

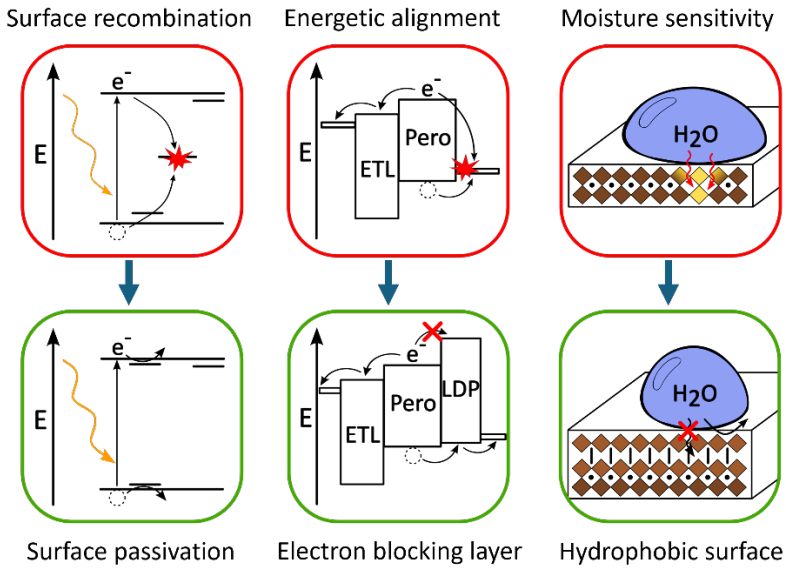

Figure 1: LDPs increase the performance of perovskite solar cells by passivating the surface (left), acting as a hole blocking layer (middle) and increasing the tolerance against moisture (right).

In this work, LDPs containing four different ammonium spacer ions have been employed as surface passivation layer on top 3D-perosvite bulk photoabsorbers. The quality of surface passivation was determined by measurements of the luminescence quantum yield and performing hyperspectral photoluminescence imaging. Additional analysis of scanning microscopy images allows assessing and comparing the surface morphology.

References:

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Decarboxylative Arylation yields novel β-Amino Acids via Nickel Photoredox Catalysis

Tim S. Stamp,[1] Ning Wei,[1] Sebastian B. Beil[1]

[1] *Max-Planck-Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany*

Over the past decade, visible-light metallaphotoredox catalysis was able to combine iridium based photo radical generation with the robust cross-coupling potential of classical transition metal catalysis.[1–3] This mild dual catalytic approach has significantly expanded the modern synthetic toolbox of organic chemists, utilizing a variety of readily available functional groups, as well as improving sustainability and step economy.

Natural α-amino acids serve as abundant and renewable feedstock chemicals bearing a carboxylic acid group.[4] Upon single electron oxidation via the excited state iridium photocatalyst, the carboxylic acid is able to undergo efficient decarboxylation, generating a highly reactive, nucleophilic, carbon centered radical. This easily adds to a cost-effective nickel catalyst and undergoes subsequent C–C coupling reactions.[5]

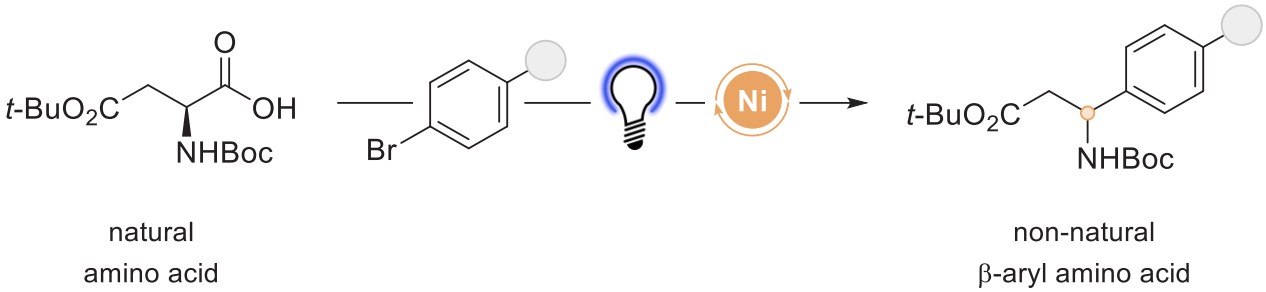

Figure 1: Arylation of natural amino acids via nickel photoredox catalysis forming non-natural β-aryl amino acids.

Our group, after optimization and mechanistic investigation, was able to utilize aspartic acid and couple it effectively with a broad range of electron poor aryl bromide, giving the respective products in good yields. Included in the scope is a broad range of singularly substituted aryl bromides, as well as pharmaceutically relevant motives and functional groups facilitating post modification.

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Functional characterization of the *C. elegans'* mitochondrial 2-ketoacyl-CoA thiolase (*kat-1*) using comparative metabolomics

Marie-Désirée Schlemper-Scheidt [1], Siva Bandi [1], Stephan H. von Reuss [1]

[1] *Université de Neuchâtel, Institute of Chemistry, Neuchâtel, Switzerland*

Mutation of the mitochondrial 3-ketoacyl-CoA thiolase (*kat-1*) shortens *C. elegans* lifespan but its function remains enigmatic.[1]

Comparative metabolomics of C. elegans wild-type (N2) and *kat-1(tm1037)* highlighted *kat-1* enriched (Fig.1). Their NMR characterization revealed a diversity of modular glucosides (MOGLs) with tiglate as common feature, suggesting that *kat-1* is involved in tiglic acid metabolism. Incorporation experiments utilizing an *E. coli Δile Δleu Δval* mutant as bacterial food source that could be specifically enriched with either L-[U-$^{13}C_5$]-valine, L-[U-$^{13}C_6$,^{15}N]-leucine, or L-[U-$^{13}C_6$,^{15}N]-isoleucine highlighted metabolites derived from branched chain amino acid metabolism. Tiglate units of the *kat-1* enriched MOGLs were specifically [$^{13}C_5$]-enriched upon incorporation of L-[U-$^{13}C_6$,^{15}N]-Ile, identifying it as 2-methylacetoacetyl-CoA thiolase in mitochondrial L-isoleucine metabolism. Free *anteiso*-C5 acids upstream of 2-methylacetoacetic acid, such as nilic acid and tiglic acid, were also [$^{13}C_5$]-labelled upon incorporation of L-[U-$^{13}C_6$,^{15}N]-Ile and strongly enriched in *kat-1*. An increased flux of *anteiso*-C5 building blocks from mitochondria was characterized by ESI-(+)-MS^E screening for *O*-acyl carnitines, which demonstrated that *O*-nilate-L-carnitine, *O*-tigloyl-L-carnitine, and *O*-2-methylbutyryl-L-carnitine are strongly enriched in *kat-1*. Furthermore, mutations in *glo-1(zu391)*, *glo-3(kx94)*, and *glo-4(ok623)*, essential for lysosome-related organelle (LRO) formation, demonstrated suppresstion of tiglate-substituted MOGL formation.[2,3]



Figure 1: Comparative metabolomics of *C. elegans* wild-type (N2) and *kat-1*.

Here we provide a functional characterization of *kat-1* as mitochondrial 2-methylacetoacetyl-CoA thiolase and demonstrate that mitochondrial L-Ile metabolism provides tiglate building blocks, exported via the carnitine shuttle and utilized for the biosynthesis of MOGLs in LROs. How this pathway results in the reduced lifespan of *kat-1(tm1037)* remains to be identified. Consequently, *C. elegans kat-1* represents a potential model system for mitochondrial acetoacetyl-CoA thiolase (T2) deficiency, a rare human disease. [4]

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An economic-chemical view of the global distribution of raw materials, resources and reserves for the production of Sodium-Ion Batteries

Niklas Padberg[1]

[1] *University of Münster, Institute of Business Chemistry, Münster, Germany*

Sodium-Ion Batteries (SIBs) are promising alternatives to Lithium-Ion Batteries (LIBs) in some market segments. In addition to lower material costs, they also promise reduced dependencies. With the rapid development of competitive SIBs, cost structures and the value chain are becoming increasingly important[2]. However, little research has been done on these areas to date. This paper provides a comprehensive analysis of raw material reserves and resources. This allows the total costs of SIBs to be determined in a cost model[3].

At present, there are various options for the cell chemistries of Sodium-Ion Batteries that show promise for market readiness[4]. These require different raw materials and different processing steps. This work takes a closer look at the global distribution of resources and reserves. Based on this, possible value chains are identified, all the way to the finished battery. With a particular focus on the potential for establishing more resilient supply chains, possible location scenarios in the US, Europe, and China are developed and discussed.

In this study, it's also looked at what the raw materials are currently used for and how demand might change if SIBs get a bigger share of the market. To do this, critical raw materials are examined further, and potential bottlenecks are identified. Ways to deal with shortages in the supply of raw materials are also pointed out.

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Computationally assisted engineering of urethanase activity

Niklas Rimkus,[1] Jan Mican,[2] Joan Planas,[2] David Bednar,[2] Jiri Damborsky,[2] Thomas Bayer,[1] Uwe T. Bornscheuer [1]

[1] *University of Greifswald, Institute of Biochemistry, Greifswald, Germany*
[2] *Masaryk University, Loschmidt Laboratories, Brno, Czech Republic*

To address the accumulation of (post-consumer) plastic waste in the environment, advanced and sustainable recycling methods are greatly demanded.[1,2] While the enzymatic depolymerization of polyesters has been targeted in the past, efficient recycling strategies for polyurethanes (PUs) are still elusive.[3] Although the first enzymes acting in highly stable carbamate bonds were discovered recently, their intrinsic properties need to be improved substantially to become industrially relevant.[4-6]

In this study, computational tools including molecular dynamics simulations, ancestral sequence reconstruction, and flexibility predictors were utilized to enhance thermostability, organic solvent tolerance, and long-term shelf-life of urethanases by >7-fold compared to previously described wild-type enzymes. Improved urethanases also exhibited up to 6-fold higher activity against the commercial polyester-PU Impranil®. Finally, the results aided the elucidation of sequence-structure-function relationships, which will guide future engineering campaigns.

Together, this study highlights the potential of complementary computational tools to accelerate the development of a sustainable processes for PU recycling and beyond.

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Polydentate, binucleating Ligands for Cu(I) dioxygen adduct formation

Lars. A. Georg[1], Luisa K. Träger[1], Sigfried Schindler[2], Richard Göttlich[1]

[1]*Justus Liebig University, Institute of Organic Chemistry, Giessen, Germany*

[2]*Justus Liebig University, Institute of Inorganic Chemistry, Giessen, Germany*

The efficient and sustainable usage of **oxidation processes** is among the most important challenges for modern chemistry. The established processes often rely on environmentally harmful chemicals and/or energy intensive conditions.[1] Molecular dioxygen (O_2) constitutes the most attractive green oxidant; however, its kinetic stability severely limits its direct and selective application.[2] Henceforth **biomimicing** enzymes, copper complexes can be used for activating dioxygen by forming a variety of adducts, which correspond to a wavelength of absorbance.[3]

In this work, the entropic penalty associated with adduct formation and the steric environment were systematically modulated through the use of binucleating ligands. By bridging two tmpa (N,N,N′,N′-Tetrakis(2-pyridylmethyl)ethylenediamine) motifs and varying the bridging backbone, stable yet reactive copper–dioxygen adducts were obtained, rendering them suitable for the oxidation of a range of substrates. Stopped−flow UV/Vis measurements are shown in Fig. 1. This study demonstrates binucleating ligand design as an effective strategy for tuning ligand architecture and reactivity.

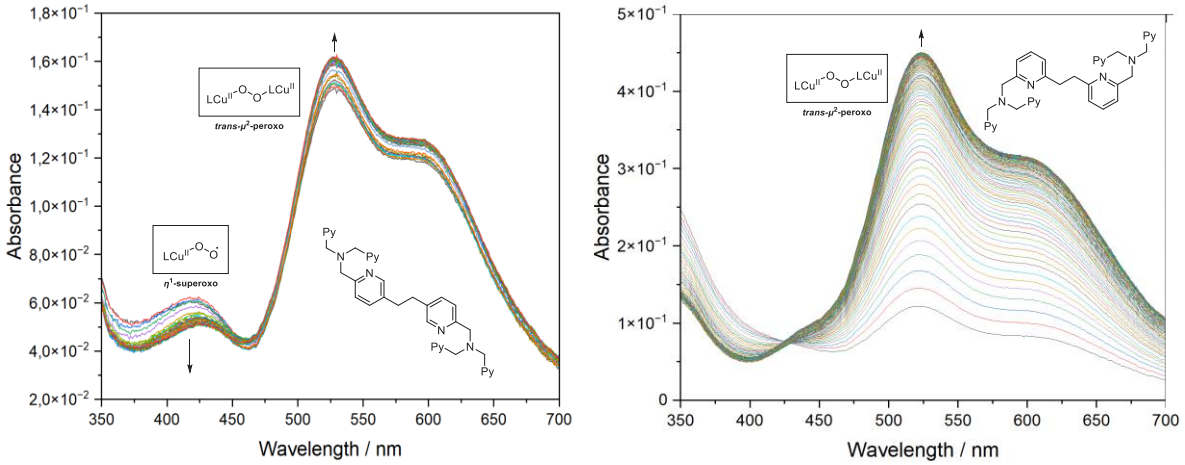

Figure 1: Binucleating ligands and their absorbance bands associated with copper dioxygen adducts.

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Young Chemists Network (JCF) Bayreuth

Jonas Schnau[1]

[1] *University of Bayreuth, Bayreuth, Germany*

The JungesChemieForum Bayreuth, a local chapter of the German Chemical Society (GDCh), was established in 2013 and organized numerous events until the COVID-19 pandemic. During the pandemic, JCF activities largely came to a halt, with only a few scientific lectures taking place. In December 2023, the JCF was re-established and has since grown to 16 active members. Over the past two years, the JCF Bayreuth has offered various types of lectures, excursions, and seminars.

These events attracted large audiences, in some cases even filling lecture halls beyond capacity. The JCF Bayreuth members, all eager to participate in organize events, invite speakers, represent the JCF on social media and contributing their own ideas tot he local chapter.

A core element of the JCF Bayreuth consists of well-attended scientific lectures delivered by distinguished researchers from academia. These talks covered a broad spectrum of contemporary chemical research, including materials and polymer science, environmental and exposure chemistry, and future energy storage technologies such as lithium metal batteries. In addition, popular science lectures by Prof. Klaus Roth and an experimental show by Erik Siemes attracted large audiences, in some cases exceeding 200 participants, thereby fostering enthusiasm for chemistry beyond the immediate academic community.

To specifically support early-career development, the JCF Bayreuth organized practice-oriented workshops, including training in scientific report and protocol writing in both German and English, as well as career-focused workshops addressing pathways to internships, scholarships, and PhD positions at leading international universities. These events equipped participants with essential transferable skills relevant to both academic and industrial career paths.

Furthermore, excursions to industrial partners such as BASF in Ludwigshafen, to the Kulmbach brewery, and to the international K Trade Fair in Düsseldorf offered valuable insights into industrial research, development, and production processes.

Overall, the activities of the JCF Bayreuth in 2024 and 2025 made a significant contribution to scientific education, career development, and networking of young chemists, establishing the chapter as a central platform for engagement and exchange at the University of Bayreuth.

Is it possible to coordinate two metal centers via a bis(amino)acetylene ligand?

Malte-Joseph B. Reihwald,[1] Lorenz Crome,[1] Wolfram W. Seidel[1]

[1] *University of Rostock, Institute of Chemistry, Rostock, Germany*

Donor-substituted alkynes are capable of serving as bridging ligands to form polynuclear complexes, with d^6-metals proving particularly suitable for this purpose. Various binding modes are possible, with the *side-on* coordination being of special interest due to its bent geometry, which facilitates an exceptionally short distance between the coordination centers. This enables cooperative electronic behaviour of the two centers, which can be studied using spectroscopic and electrochemical methods.

Polynuclear complexes of this binding mode have already been reported for sulfur, phosphorus, and carbon, some of which exhibit interesting redox chemistry and catalytic activity.[1] However, the formation of a polynuclear complex utilizing two nitrogen atoms as donors has not yet been achieved and is the objective of these investigations. However, free bis(amino)acetylene is not accessible as a ligand due to intrinsic instability caused by proton migration. To synthesize a side-on-coordinated alkyne complex, an alternative approach must be pursued. One possibility was demonstrated by LIPPARD *et al.*, who achieved the reductive coupling of two carbon atoms of isocyanide ligands using an excess of zinc.[2] This coupling was also achieved through the use of nucleophilic reagents or Br_2 by FILIPPOU *et al.*.[3]

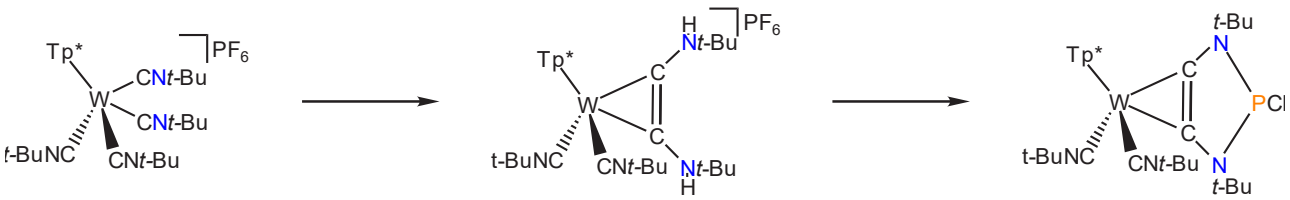

Figure 1: Synthetic pathway to a possible bridged bis(amino)acetylene complex.

Following successful coupling and subsequent deprotonation, reactivity studies with phosphorus trichloride were conducted. For this, the work of BURCK *et al.* on the reaction of diazadiene with PCl_3 to form an *N-P-N* structural unit served as the basis for planning the reaction.[4]

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A Diastereoselective Synthesis of small αα Calix[4]pyrrole Building Blocks

Clara Schritt[†1], Janos Wasternack[†1], Friedrich Braune[1], Sebastian Müller[1], Carlo Fasting[1], Daniel Bombei[1], Siegfried Eigler[1] and Christoph A. Schalley[1*]

[1] *Freie Universität Berlin, Institut für Chemie und Biochemie, Berlin, Germany*

Two-walled αα calix[4]pyrroles are versatile anion- and ion-pair receptors that are used in supramolecular assemblies and functional materials.[1] Their preparation commonly proceeds via the statistical formation of a mixture of αα/ab calix[4]pyrrole diastereomers and subsequent separation of the diastereomers.[2] Since most applications only use the αα diastereomer, the αβ diastereomer usually goes to waste. The chromatographic separation of the statistical mixture of diastereomers is challenging for calix[4]pyrroles with aromatic walls and was not yet reported for calix[4]pyrroles with aliphatic *meso*-substituents.

In this work, we have studied different approaches to the isolation of αα calix[4]pyrroles.[3] First, the issue of chromatographic separability was addressed. A chromatographic method for the separation of calix[4]pyrrole diastereomers was developed.

To obtain small two-walled αα calix[4]pyrrole building blocks on a synthetically useful scale, we developed a diastereoselective synthesis. Method-optimization led to high yields of αα calix[4]pyrroles. The versatility of the synthesis was demonstrated by the preparation of different targets. Further, methods for chemoselective post-functionalization of those αα calix[4]pyrrole building blocks enable their implementation within functional materials.

With this study, we want to kick start the development of more controlled diastereoselective calixpyrrole syntheses and deliver access to versatile building blocks for complex molecular architectures.

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A Scalable and Resource-Saving Synthesis of Dipyrromethanes and Tetrapyrroles - Minimal Polymer Formation and Facile Purification

Janos Wasternack[a]*, Clara Schritt[a], Luca Steiner[a], Ole Specht[a], Friedrich Braune[a], Marius Balizs[a], Sebastian Müller[a], Anja Wiesner[a], Beate Paulus[a], Siegfried Eigler[a] & Christoph A. Schalley[a]*

[a] *Institut für Chemie und Biochemie, Freie Universität Berlin, 14195 Berlin, Germany*



Figure SEQ Figure * ARABIC 1: Cleaner path towards dipyrromethanes and tetrapyrroles.

Dipyrromethanes and **tetrapyrroles** are important **building blocks** in material sciences, selective adsorbents and filters, medicinal chemistry, bioimaging and photocatalysis with fluorescent dyes and supramolecular chemistry. Their synthesis often is a **bottleneck** in their application, with common hurdles being extensive polymer formation, limited functional group tolerance, low yields and poor scalability.[1–4] We present an **improved** methodology for the **synthesis** of dipyrromethanes and tetrapyrroles. A key improvement is the drastic **reduction of polymerization** which highly simplifies purification, either by recrystallization or short column chromatography. Also, the **mild conditions** put forth excellent yields and a high functional group tolerance.[1] Key advantages of the new procedure are: Drastically **reduced consumption** and efficient **recycling** of pyrrole leading to **cost savings**. The new protocols deliver high yields and high-purity products. **Scale-up** preparation of dipyrromethanes was performed on 1000 mmol scale and of tetrapyrroles on 250 mmol scale. The procedure will be useful in a broad field of **applications within functional materials**, particularly in the emerging field of C[4]P-based materials. Versatile electrophilic and nucleophilic building blocks with **synthetic anchors** were obtained on **multi-gram scale.** In total, **27 dipyrromethanes** and **20 tetrapyrroles** have been prepared, covering a **wide range of functional groups** and reactivity types.

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Colourful Pertechnetates: From Simple Salts to Subtle Bonds

Clarence Yong,[1] Dennis Grödler,[2] Antonio Frontera,[3] Erik Strub[1]

[1] *University of Cologne, Division of Nuclear Chemistry, Cologne, Germany*
[2] *Helmholtz-Zentrum Dresden-Rossendorf, Resource Ecology, Dresden, Germany*
[3] *University of the Balearic Islands, Department of Chemistry, Palma, Spain*

Pertechnetate, $[TcO_4]^-$, is described as a simple, colourless tetrahedral anion mainly serving as a reference point in technetium chemistry. A closer look at its solid-state chemistry, however, reveals a surprisingly rich and colourful picture. Here, we present recent findings from our group that highlight how pertechnetates can engage in subtle yet structurally meaningful interactions, progressing from classical metal salts to more complex assemblies.

We begin with a broad survey of metal pertechnetates spanning large parts of the periodic table, including alkali-earth metals, 3d transition metals, group 12 elements, and lanthanides.[1] Despite their apparent simplicity, these compounds form well-defined crystals with diverse packing motifs, as revealed by single-crystal X-ray diffraction. Within this family, close Tc···O contacts are observed in selected structures that are consistent with matere bonding, indicating that directional interactions can be present in otherwise classical salts.[2]

The structural chemistry becomes even more expressive with crown ethers. In potassium crown ether systems, the pertechnetate anion forms pronounced directional interactions with the K^+–crown complex, leading to distinctive structural motifs.[3] Finally, we present results on rubidium pertechnetate crown ether compounds, where dimeric assemblies feature intramolecular matere bonds.[4] These findings, illustrate how weak interactions can be reinforced and organised through careful choice of counterions and ligands.

Vividly coloured crystals and elegant ORTEPs highlight the theme of Colourful Chemistry and show how pertechnetates combine visual appeal with subtle bonding phenomena.

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Sustainable Design-Oriented Biopolymeric Platforms for Visual pH Sensing

Veselina Adımcılar

Istanbul Technical University, Department of Chemistry, Istanbul, Türkiye

The growing demand for cost-effective and sustainable chemical sensor materials for real-time monitoring of environmental changes has shifted researchers focus toward employing plant-derived sources namely biopolymers combined with natural pigments.[1] These innovative systems particularly plant-based systems have attracted attention due to their renewable origin, environmentally friendly nature, bioactive properties and versatility and adaptability to form different matrices which can be used for various purposes. Among these, pH-responsive materials that respond to the chemical changes through color shifts offer an on-site and instrument-free monitoring of chemical conditions relevant to food quality, medical and environmental safety related applications.[2-4]

In this study, a design-oriented and plant-based biopolymeric sensing platform exhibiting high color sensitivity toward pH variations is developed and characterized. The pH-sensitive properties of the developed system are obtained from the presence of natural anthocyanins from plants, incorporated in the biopolymeric matrix, capable of undergoing sharp, distinct, and detectable color change within a wide range of pH. The platform is engineered to function in different design configurations, and physical formats allowing assessment of the influence of structural form on physical integrity, stability, and functional performance. In addition to its sensing capability, the contribution of seed-derived and plant-based components to the bioactive properties of the platform is also studied. The incorporation of bioactive plant materials enhances the antioxidant activity of the platform, supporting its classification as an active material. The findings highlight the versatility of the developed biopolymeric platform and its potential applicability in sustainable, real-time pH monitoring applications through vivid color changes.

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Best Supervisor Award – Award for excellent supervision

Awardee: Prof. Dr. Lena Daumann[1]

Laudatio: Pia Heinrichs[1]

Organizer: JCF Team Science & Education

[1] *Institute for Bioinorganic Chemistry, Heinrich-Heine-Universität Düsseldorf, Germany*

The quality of supervision during doctoral studies is a decisive factor for the scientific success, motivation, and personal well-being of doctoral candidates. The Young Chemists Forum (JCF) of the GDCh is actively committed to improving doctoral conditions in the long term. A central component of this is the Best Supervisor Award. This award recognizes supervisors who, through their exceptional commitment and modern leadership culture, serve as role models for the scientific system. The aim is to highlight excellent supervision and reinforce the principle that good supervision should be the rule, not the exception.

This year, the jury is honouring Prof. Dr. Lena Daumann for her outstanding and holistic approach to supervision. She impressed with a comprehensive package that goes far beyond technical mentoring.



Figure 1: Awardee of the Best Supervisor Award 2026: Prof. Dr. Lena Daumann

Her crisis management and empathy are particularly noteworthy: during the relocation of her research group, she found individual solutions for all doctoral students to enable them to continue their doctoral studies smoothly at the old location. In addition, Prof. Daumann, backed by her qualification as a mental health trainer, proactively integrates the promotion of mental health and the compatibility of family and career into her leadership style.

Her supervision concept is also characterized by excellent structural conditions, including regular development meetings and the targeted promotion of soft skills for career paths within and outside the academy. With her clear commitment to diversity, inclusion, and the FAIR principles, Prof. Dr. Lena Daumann exemplifies the values of responsible, modern, and humane supervision in chemistry.

Paleobiotechnology: Using ancient DNA for natural product discovery

Sabrina Even, [1,2] Alexander Gale,[1,2] Martin Klapper,[2] Rosa Herbst,[2] Yusuke Hioki,[2,3] Judith Boldt,[2] James Fellows Yates,[2,5,6] Alexander Hübner,[5] Christina Warinner,[4-6] Pierre Stallforth[1,2]

[1] Friedrich-Schiller-University Jena, Faculty of Chemistry and Earth Sciences, Jena, Germany

[2]Leibniz Institute for Natural Product Research and Infection Biology – Hans-Knöll-Institute, Department of Paleobiotechnology, Jena, Germany

[3] School of Pharmaceutical Sciences, University of Shizuoka, Japan

[4] Harvard University, Department of Anthropology, Cambridge, Massachusetts, United States

[5] Max Planck Institute for Evolutionary Anthropology, Department of Archaeogenetics, Leipzig, Germany

[6] Leibniz Institute for Natural Product Research and Infection Biology – Hans-Knöll-Institute, Department of Archaeogenetics, Jena, Germany

The search for structurally diverse bioactive small molecules has highlighted microorganisms as prolific producers of low-molecular-weight natural products. Accordingly, microbial metabolites have become central targets of research for expanding the repertoire of compounds accessible for biomedical and biotechnological applications. In light of the growing global threat of antimicrobial resistance, there is an urgent need to broaden the pipeline of therapeutics and to access new chemical space. [1] To address this, innovative approaches including the novel field of Paleobiotechnology have emerged. This research area combines metagenomic analyses of ancient DNA with genome mining thus introducing the dimension of time into natural product discovery.[2]

Rather than restricting our search to contemporary microbiomes, we examine the genetic information preserved in ancient microbial communities through sources of bacterial DNA, including dental calculus from prehistoric specimens.[3,4] By reconstructing metagenomes from these ancient samples, we can identify biosynthetic genes that may yield previously undiscovered bioactive compounds. These genes are subsequently expressed in modern microbial chassis for functional and structural investigations.[3]

Our research employs state-of-the-art technologies for both metagenome assembly and functional gene analysis, as well as for the identification and isolation of the finally synthesized natural products.[3,4] We further expand our field of investigation by exploring traditionally produced foods from regions that have remained largely unaffected by modern industrial practices, which may provide an additional rich source of novel bioactive natural products.[5]

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Spin-State Photoswitching in a [5]Helicene-Based Hydrocarbon

Takuma Miyamura,[1] Lukas Jacob,[2] Philipp Thielert,[3] Sabine Richert,[3] Stefano Crespi,[2] Oliver Dumele[1]*

[1] *University of Cologne, Institute of Organic Chemistry, Cologne, Germany*
[2] *Department of Chemistry, Uppsala University, Sweden*
[3] *University of Freiburg, Department of Chemistry, Freiburg, Germany*

Precisely controlling the spin state of molecular entities in a reversible manner is one of the longest standing challenges and motivations for scientists. It is especially challenging for stable and purely organic molecules because they are usually locked in a closed-shell electronic configuration.[1,2]

This contribution focuses on the development of helical photochemical spin-state switches.[3,4] Initially, 1,14-(±)-dimethyl[5]helicene was used in designing a photochemical switch with (meta)stable spin states. By introducing dimethylanthryl substituents at the 4th and 11th positions, the [5]helicene core undergoes photochemical retroelectrocyclization to form a paramagnetic species (**1**-O, **Figure 1**). The back reaction to its initial form **1**-C can be triggered thermally or by quantum tunnelling at cryogenic temperatures. At high temperatures, a unidirectional rotational motion has been confirmed, making this system a unique spin-state photoswitch with light-driven molecular motor properties.

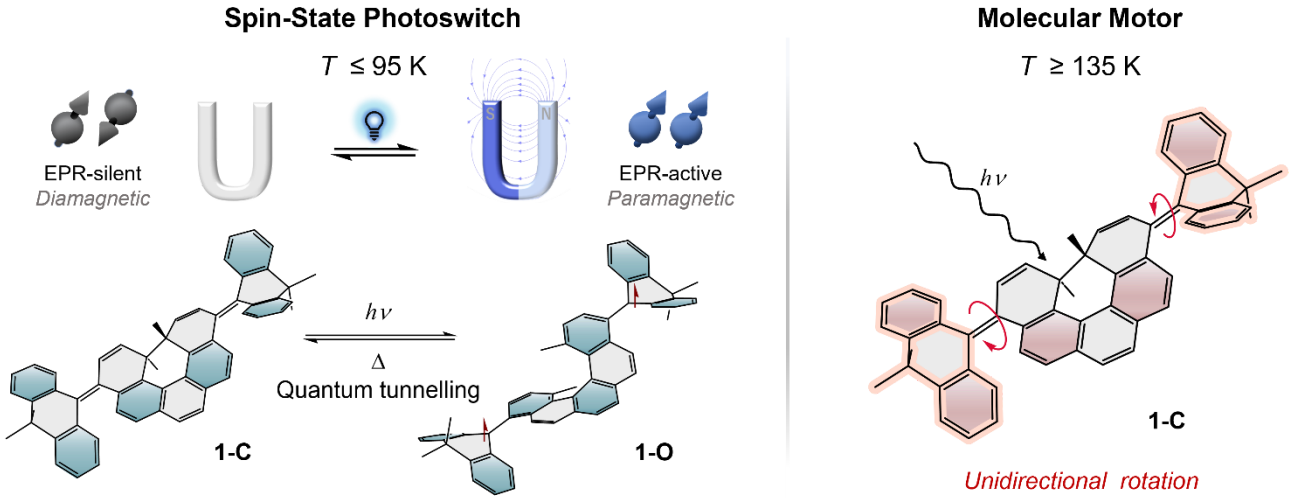

Figure 1: Photo- switching (left)/isomerization (right) of **1** in different temperature ranges.

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Recovery of Germanium from Germanium Dioxide Using Hydrogen or Natural Gas in Chemical Vapour Transport Processes

Julian Burkhart, [1] Christian A. Bömer, [1] Jana Milanovic, [1] Victoria S. Drescher, Igor Atanasov, [1] Moritz Maxeiner, [1] Klaus Müller-Buschbaum[1]

[1] *Justus-Liebig-University Giessen, Institute of Inorganic and Analytical Chemistry, Giessen, Germany*

Germanium (Ge) is a critical element extensively used in advanced technologies, such as optical fibres, infrared optics, polymerisation catalysts and semiconductor devices.[1,2] This study investigates the recovery of germanium from germanium dioxide (GeO_2) via chemical vapour transport (CVT), using hydrogen or natural gas as transport agents. The work aims to optimise key reaction parameters, including gas composition, temperature gradient and gas flow rate, in order to maximise germanium yield while minimising energy demand. Experimental results indicate that both hydrogen and natural gas efficiently promote the reduction to the volatile transport species germanium monoxide (GeO), leading to the deposition of Ge and GeO_2 at the sink. The use of hydrogen enables an environmentally-friendly reduction with a high reducing potential, which requires adjustments in the gas composition to achieve optimal recovery conditions. In contrast, natural gas provides economic benefits due to its widespread availability. However, its application involves sustainability and operational challenges, such as carbon dioxide (CO_2) emissions and carbon deposition, which affects product purity, process efficiency and environmental performance. These aspects highlight the necessity of balancing process efficiency with environmental impact when selecting an appropriate transport agent. Overall, the results using hdyrogen present an efficient and sustainable approach for germanium recovery, supporting the circular economy and reducing dependence on primary germanium resources.

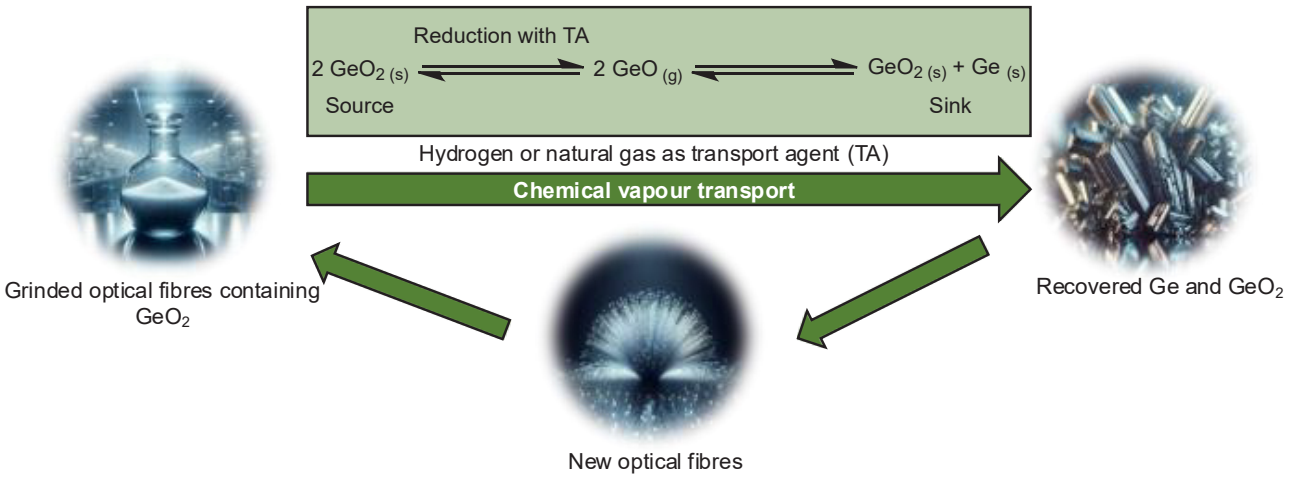

Figure 1: Schematic life cycle of GeO_2-containing optical fibres using CVT recovery method. This picture was partly created with AI (engine: Adobe Firefly).

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P70

Targeting fibrin with EPep: A peptide probe for stroke research

Philipp Holz[1], Dmitrii Antuganov[2], Qinyu Wang[3], Lukas Vieth[3], Bernd Neumaier[2,3], Heike Endepols[3], Holger Grüll[3], Ines Neundorf[1]

[1] University of Cologne, Institute of Biochemistry, Cologne, Germany.
[2] Research Center Jülich, Institute of Neuroscience and Medicine, Jülich, Germany.
[3] University Clinic Cologne, Institute for Diagnostic and Interventional Radiology, Cologne, Germany.

Thrombosis, defined by the intravascular formation of fibrin-rich clots, is a major driver of stroke and other ischemic thrombi worldwide. It remains a leading contributor to global morbidity and mortality. Early detection and precise localization of fresh thrombi are crucial for timely intervention. Conventional imaging modalities such as CT or MRI are often limited in identifying small or evolving infarcts. Molecular imaging with fibrin-specific probes offers the sensitivity and specificity needed to visualize thrombus formation at the biochemical level. Our overarching goal was to develop a biocompatible PET/SPECT tracer capable of early thrombus detection, real-time monitoring of clot evolution, and longitudinal assessment of therapeutic outcomes in preclinical models.

Based on the EP2104R peptide[1], we designed EPep: a cyclic, fibrin-targeting peptide probe incorporating unnatural amino acids and a stabilizing disulfide bridge. These structural features enhance binding affinity, proteolytic resistance, and *in vivo* stability.[2] EPep was synthesized via a combination of automated and manual solid-phase peptide synthesis, ensuring sequence fidelity and high yields. For multimodal imaging, a NOTA chelator was appended to facilitate radiolabeling with ^{68}Ga and Al^{18}F under mild conditions. *In vitro* assays investigated hemolytic activity and stability in human serum. *In vivo* evaluation in a mouse model of arterial thrombosis revealed rapid and specific accumulation of radiolabeled EPep at clot sites, with high target-to-background ratios. Ongoing investigations extend these promising findings in other thrombosis models to further characterize probe pharmacokinetics and imaging performance.

Collectively, our data underscore the potential of EPep derivatives as high-performance imaging agents for early detection and longitudinal monitoring of thrombotic and ischemic pathologies, paving the way for future clinical translation and improved patient management.

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Highly Efficient Thermally Activated Delayed Fluorescence (TADF) OLED under Strong Exciton-Photon Coupling Showing Narrowband and Tuneable Emission

Soyoung Boo[1], Andreas Mischok[1], Francisco Tenopala-Carmona[1], Julia Witt[1], Malte C. Gather[1,2]

[1] *Humboldt Centre for Nano-and Biophotonics, Department of Chemistry, University of Cologne*

[2] *SUPA, School of Physics and Astronomy, University of St Andrews, UK*

Polariton organic light-emitting diodes (POLEDs) leverage strong light-matter coupling to generate quasiparticles known as exciton-polaritons [1]. Under the right conditions, this results in narrowed and angle-independent emission compared to conventional microcavity OLEDs [2]. A promising strategy to enter the strong coupling regime is to embed the OLED stack and an assistant strong coupling layer (SCL) within a planar microcavity. The resulting upper and lower polariton branches can be controlled by adjusting optical cavity thickness, refractive index, and molecular orientation [3-5]. Despite these advances, realizing POLEDs with efficiencies comparable to state-of-the-art TADF OLEDs remains challenging.

In this study, efficient TADF POLEDs were realized using SpiroAC-TRZ as a blue TADF emitter and BSBCz as SCL, both exhibiting horizontal orientation in thin films. The resulting POLEDs showed distinct polariton branches, exhibited angle-stable emission with EQEs reaching 20% (blue) and 25% (green), and show tunable emission spectra over a range from 490 to 545 nm with the same emitter.

These results demonstrate the crucial role of orientation control in achieving efficient polariton emission and the realization of high-performance POLEDs in the sky-blue regime enables applications at industry-relevant device efficiency.

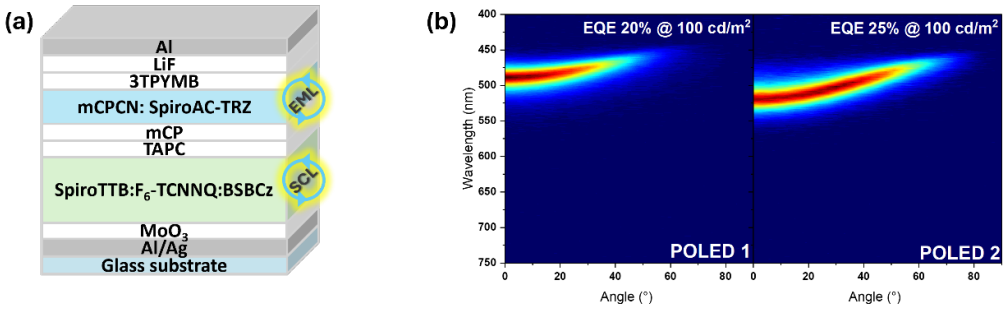

Fig. 1 (a) Device architecture of POLED with an assistant SCL, positioned at the second maximum of the electric field in microcavity. (b) Angle-resolved electroluminescence spectra with EQEs

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Illuminating Artemisinin: A Photochemical Approach to Unlock Its Pharmacological Potential Beyond Malaria

Jan F. W. van Stiphoudt,[1] Axel G. Griesbeck[1]

[1] *University of Cologne, Institute of Organic Chemistry, Greinstr. 4-6, 50939*

Artemisinin is a natural compound containing an unusual 1,2,4-trioxane *endo*-peroxide. This endo-peroxide provides the unique and important pharmacological potential of Artemisinin with the treatment of malaria being its main application. In this context, the mode of action of Artemisinin proceeds via an activating reductive homolytic cleavage of the peroxide through biologically available Fe(II)-ions. This initiates a radical cascade with several reactive oxygen species (ROS) and carbon-centered radicals. These intermediates act as alkylating agents and initiators of oxidative stress within the malaria pathogen, resulting in the death of the malaria-causing parasite through irreparable DNA damage.[1,2]

In the light of the concept of photopharmacology, we investigate a new approach to transfer this unique mode of action onto other types of diseases, e.g. cancer therapy. We found that the homolytic peroxide-cleavage can be photochemically initiated via irradiation of triplet-sensitizers or new singlet-emitters.[3]

Herein, we report the synthesis and comprehensive photophysical characterization of new xanthone- and acridone-based activators as well as molecular dyads composed of these activators and Artemisinin. We found a highly solvent-dependent fluorescence behavior concomitant with the attenuation of fluorescence in the presence of Artemisinin which we assign to an energy transfer from the excited activator onto the peroxide-motif. Additional irradiation experiments indicate a decomposition process similar to the above-mentioned Fe(II)-induced activation of Artemisinin.

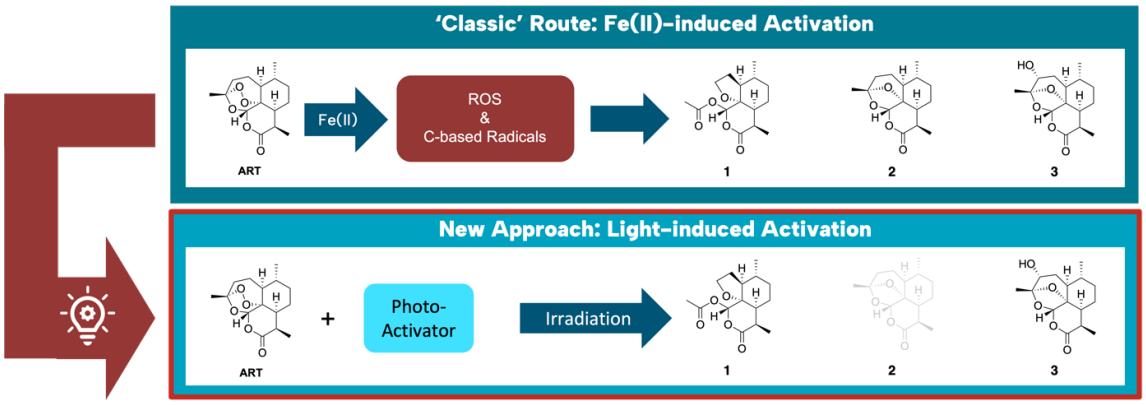

Figure 1: General concept of the Photoactivation of Artemisinin (ART). Irradiation with a suitable photo-activator leads to the same rearrangement products 1 and 3 as the known Fe(II)-induced route indication a similar reaction pathway.

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Theoretical Effect of Si and B Substitution on Physical and Magnetic Properties of Fe_2P-based Compounds

Dorothee Benedens[1], Stephan Erdmann[1], Halil İ. Sözen[1], Thorsten Klüner[1]

[1] *Carl von Ossietzky University of Oldenburg, Institute of Chemistry, Oldenburg, Germany*

Rare-earth-free Fe_2P-based magnets exhibit remarkable magnetic properties and are therefore promising candidates for a wide range of technological applications.[1] The objective of this work was to study the influence of Si and B substitution on the structural and magnetic properties of Fe_2P compounds, with particular focus on enhancing the relatively low Curie temperature of 214 K.[2,3] In this work density functional theory was used in the framework of VASP (Vienna Ab Initio Simulation Package) to obtain a systematic overview of the investigated properties. By starting from binary Fe_2P and extending to ternary $Fe_2(P,Si)$, $Fe_2(P,B)$, and quaternary $Fe_2(P,Si,B)$ systems a broad range of possible compounds was screened. The study focused on physical aspects such as preferential substitution sites and lattice parameters, as well as the magnetic moments.

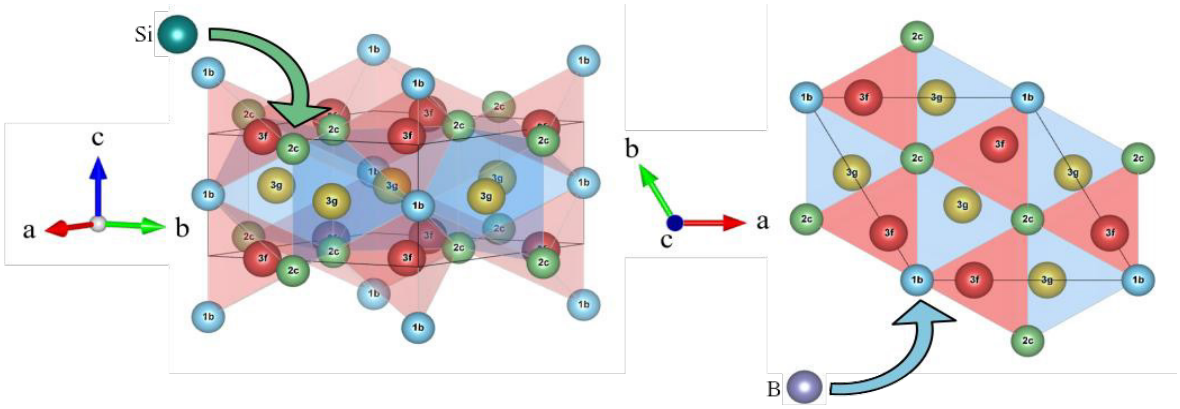

Figure 1: Depiction of the hexagonal unit cell with 3 functional units in the boundaries. In the Fe_2P structure the Iron atoms are located in the *3f* (red) and *3g* (yellow) sites, while the Phosphorous atoms are located in the *1b* (blue) and *2c* (green) sites.

Theoretical calculations reveal that the *2c* position is the preferred substitution site for Si[4], while B is expected to occupy the *1b* site. The analysis of the lattice parameters shows an increase of the lattice constant *a* and a decrease of *c*, which results in an overall decrease of the cell volume. The magnetic moments on the other hand increase with higher B and Si concentrations. The investigated effects show that substitutions of Silicon and Boron can improve the magnetic properties of Fe_2P in a way, that these magnets could proof to be possible re-free alternatives to established magnets.

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Coumarin chromophores for photoinduced activation of Artemisinin

Hannah L. Dochtermann,[1] Axel G. Griesbeck[1]

[1] *University of Cologne, Department for Chemistry and Biochemistry, Institute of Organic Chemistry, Cologne, Germany*

Artemisinin **1** (ART) is a natural product which has shifted the paradigms to combat malaria.[1,2] The combination of physiological tolerability and high potency make ART a good candidate for non-malarial applications, and its anticancer activity has captured a great deal of attention.[3] Under physiological conditions, ART is activated by Fe(II) via single electron transfer (SET) to the endoperoxide bond, generating reactive oxygen radicals. These radicals undergo distinct rearrangements depending on the initial Fe(II) coordination site, ultimately forming three major products which indicate an activation via the pharmacologically relevant intermediates (Figure 1). Recent investigations[4], uncovered a novel approach to activate ART upon a remote and precise trigger – by light.

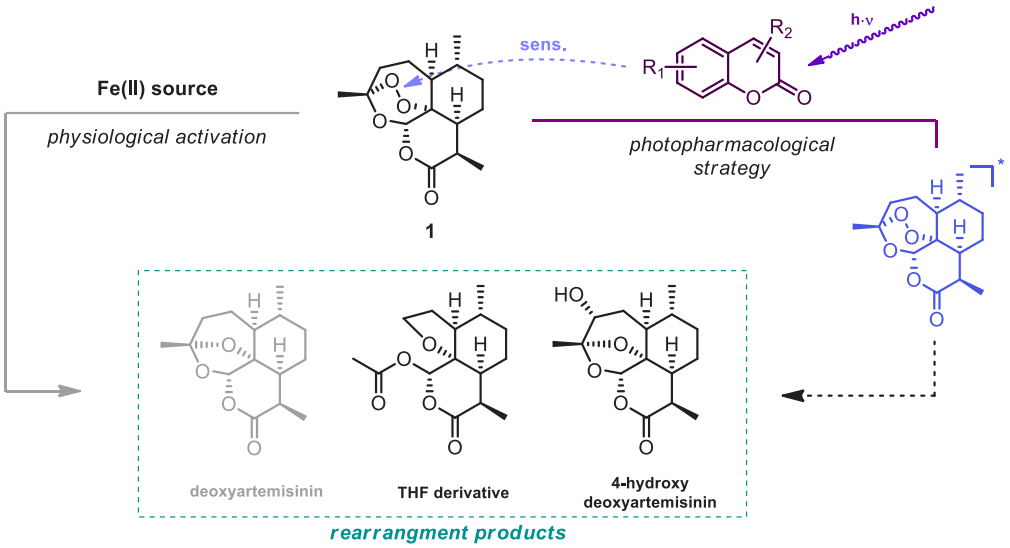

Figure 1: Novel photopharmacological strategy using coumarin derivatives to activate Artemisinin **1** which rearranges to shown products (deoxyartemisinin is not generated by the light-induced rearrangement).

This novel photopharmacological strategy is based on the conjugation of ART with chromophores capable of activating the pharmacophore in the desired fashion, presumably via energy transfer. In current investigations, fluorescent coumarins are successfully employed as chromophores whose photophysical characteristics can be fine-tuned by distinct structural changes allowing for the activation of ART by light in the visible region and ultimately, paving the way for photopharmacological applications (Figure 1).

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Phase Stability and Thermodynamic Properties of Magnesium Carbonates in Salt Solutions

Hagen Fiebig,[1]

[1] *TU Bergakademie Freiberg, Institute of Inorganic Chemistry, Freiberg, Germany*

The long-term safety assessment of radioactive waste repositories is largely based on thermodynamic modelling, which requires a robust understanding of chemical equilibria between host rock components, saline pore fluids, waste inventories, and engineered barrier materials. In particular, carbonate concentration and *pH* exert a strong control on actinide solubility, independent of the host rock. In current rock-salt-based proposals, these parameters are planned to be actively influenced by the addition of MgO or $Mg(OH)_2$ respectively, which bind CO_2, ensure a basic *pH* of brines, and promote carbonate formation. So far however, the stability and transformation behavior of magnesium carbonate phases under repository-relevant ionic strengths remain insufficiently understood.

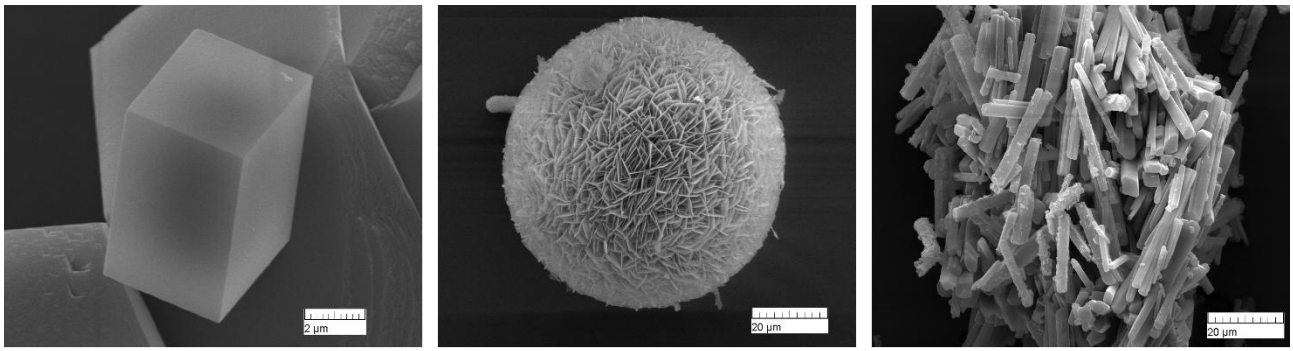

Figure 1: SEM images of prepared solids; magnesite, hydromagnesite, and nesquehonite.

Current studies are thus focused on the exploration of any chemical equilibria involved in the system Mg^{2+}–Cl^-–OH^-–CO_2–H_2O, aiming to expand the Thermodynamic Reference Database (THEREDA).[1,2] The solid magnesium carbonate phases magnesite ($MgCO_3$), nesquehonite ($MgCO_3 \cdot 3\ H_2O$), hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4\ H_2O$), dypingite ($Mg_5(CO_3)_4(OH)_2 \cdot 5{+}x\ H_2O$), and chlorartinite ($Mg_2(CO_3)Cl(OH) \cdot x\ H_2O$) have been deemed most relevant, and experimental procedures have been established that reproducibly lead to well-defined solids, as characterizations using P-XRD, SEM (e.g. Fig. 1), Raman, and TG-DSC have shown. Going forward, experimental setups will be developed to quickly establish equilibria with $MgCl_2$ solutions of differing concentrations at a given temperature and subsequently quantify the composition of the liquid and gas phases. A crucial aspect is determining the types and amounts of ionic species present, as well as their interactions in solution. As very low concentrations ($b < 10^{-5}$ mol kgw^{-1}) of CO_3^{2-} and OH^- complexes are expected, special analytical methods need to be explored.

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Optical Temperature Sensing using Metal-Organic Frameworks

Victoria S. Drescher,[1] Klaus Müller-Buschbaum[1]

[1] *Justus-Liebig-University, Institute of Inorganic and Analytical Chemistry, Giessen, Germany*

The ability to detect temperature is important in many situations. For example, it can be used to check the temperature of food, medicines or electrical devices to prevent them from spoiling or overheating, or in industrial processes. Alternative technologies are needed because conventional thermometers often reach their limits. A fast and efficient detection of temperature is made possible by optical sensors, which have the potential for a high size reduction. These sensors rely on changes in the optical properties of materials that are at best visible to the naked eye and operate within the physiological temperature range.

Metal-organic frameworks (MOFs), which are porous three-dimensional inorganic-organic networks, are excellent temperature sensors due to their variable and additive luminescence properties. Some MOFs emit visible blue light via ligand-based emission, like in the case of 4,4'-biphenyl dicarboxylic acid.[1] An increase in temperature is expected to lead to a thermal quenching of the emission. MOF luminescence can be modified by incorporating lanthanide ions, such as Eu^{3+}, into the pores of the MOF after synthesis. The emission maximum of trivalent europium is in the red region of the visible spectrum, between 610-630 nm. This can be assigned to the $^5D_0 \rightarrow {}^7F_2$ transition of Eu^{3+}.[2] Consequently, a pink emission, which is a combination of ligand and Eu^{3+} emissions, is generated by loading the MOF with Eu^{3+} ions. A colour shift in the emission is initiated by a temperature change. As the temperature rises, a shift towards red luminescence can be observed. Conversely, cooling the sample produce a more bluish emission (Figure 1). In order to characterise materials in terms of their thermometric properties, key parameters such as sensitivity and cycling performance must be examined.

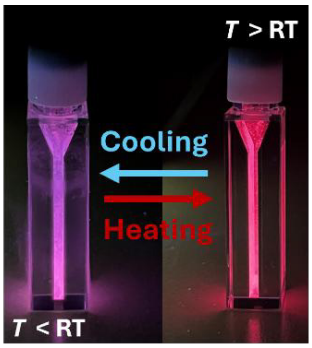

Figure 1: Temperature-dependent emission of an Eu^{3+}-loaded MOF within the physiological temperature range (RT = room temperature).

References:

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Albumin-based hydrogels and their reswelling studied by EPR spectroscopy

Felix Götze,[1] Dariush Hinderberger[2]

[1] *Martin-Luther-Universität Halle-Wittenberg, Institute of Chemistry, Halle (Saale), Germany*

Serum albumin is the most abundant transport protein in the blood of vertebrates and by this an available side-product in the industrial food production. It can be transformed into non-covalent and stable hydrogel networks, whose properties are well-suited for the embedding and controlled release of various drugs.[1,2] Due to their biodegradability and biocompatibility, these protein-based hydrogels are promising candidates for various biomedical applications such as drug delivery systems or in tissue engineering.[3]

In this project, we aim to further develop such materials made of bovine serum albumin (BSA) in order to prepare various forms of hydrogels which might be suitable for pharmaceutical approaches. Therefore, we are studying the impact of drying, grinding and reswelling on the structure and physicochemical properties of these materials. By continuous wave electron paramagnetic resonance (CW EPR) spectroscopy we are able to gain insights into the local bindings of BSA and nanoscopic structure in the formation of the hydrogels as well as the preservation of their characteristics after various treatments.

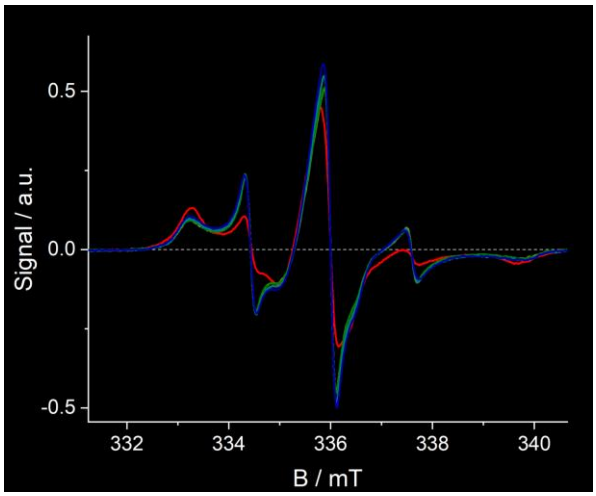

Figure 1: CW EPR spectra of spin-labeled BSA hydrogels.

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JCF – Team Science & Education

Felix Bourier[1], Johannes Voigt[2], Ekaterina Salikhova[3]

[1] *Carl Zeiss SMT GmbH, Oberkochen, Germany*
[2] *Justus Liebig University Giessen, Giessen, Germany*
[3] *Ghent University, Ghent, Belgium*

We're the Team Science & Education, a group of about 10 students and postdocs from across the JCF, scattered all across Germany. Like you we care about how our subject is taught and shared. Whether it's helping kids and pupils to find their path or helping a PhD students and beyond find their footing in science, we want share projects, tools and guidelines to make it happen.

What are we working on right now?

- For the next generation: We're designing a new experiment book for children and a "mini" version of our ChemEscape game for younger kids. We also partner with the *Grünes Klassenzimmer* to bring even more chemistry to the classrooms.
- For students & grads: We're looking into how AI is actually being used in research by organizing talks with experts in the field. Also we'‘re highlighting rare study paths you might not have considered,
- We also developed a set of PhD guidelines to provide insights into PhD funding supervisor selection and more.
- Recognizing mentorship: We organize the Best Supervisor Award to highlight the people doing it right.

Most people know us for shipping 1,500+ free ChemEscape boxes to schools, but we have a lot more cooking.

Come say hi! We're looking for new ideas and new faces. Stop by our poster at the FJS, meet the team, and have a chat with our Science-Erli & Schülerli. We'd love to hear your perspective and your contributions.



Figure 1: Science Erli, the mascot of JCF Team Science & Education.

Sustainable Chemistry - Enabling the Future!

Mirco Wende,* Kevin Keller*

**GDCh Sustainability Commission*

Chemistry stands at the intersection of today's most pressing sustainability challenges, ranging from resources and raw materials, climate crisis and environmental pollution to education and healthcare. This central position gives chemistry tremendous leverage to catalyse global sustainable development and transformation, while at the same time imposing an even greater responsibility upon us!

To address this potential and the accompanying obligation, the German Chemical Society (GDCh) has developed a sustainability strategy in response. At the core of our approach stands sustainable chemistry as a transdisciplinary guiding principle that systematically integrates ecological, social, economic and ethical responsibility throughout the entire lifecycle of chemical products and services. We base our approach on three interconnected goals: First, to activate our networks in order to pool expertise and competence, second, to jointly create knowledge about sustainable solutions through chemistry, and third, to make these resources available with added value for society, ourselves and all our stakeholders. The GDCh brings together chemists from all disciplines, enabling us to create long-term value across environmental, social and governance dimensions from diverse perspectives and to position chemistry as an enabler of sustainable solutions.

Rather than imposing directives top-down, our strategy springs from a joint effort – a collaborative development process designed to evolve dynamically with our community and its changing demands. This ensures that we maintain a stable momentum and agility in our actions while promoting interaction and engagement. At the same time, it encourages us to rethink both, the role of the GDCh and chemistry in society and to raise awareness of sustainability in chemistry. So, beyond these tasks, our strategy is not only about gathering and providing knowledge; we want to spark individual self-management, critical reflection and active participation in the transformation – rethinking chemistry is our shared responsibility!

We want to highlight our goals and the ongoing processes of our strategy implementation and demonstrate that sustainable chemistry is not an isolated discipline, but an inseparable part of the future of chemistry!

SPEAR Me, c-MYC: Toward the Structural Basis of Epigenetic Inheritance

Benno Wallwitz,[1] Daniel Friedrich[1]

[1] *University of Cologne, Department of Chemistry and Biochemistry, Cologne, Germany*

Gene activation is required for cells to respond to developmental cues, environmental signals, and changes in cellular state. This process is initiated by transcription factors that recruit chromatin modifiers and remodellers, enabling the transcription machinery to access specific genomic regions. Once activated, many genes remain active across multiple cell divisions during differentiation, organogenesis, and tumorigenesis.

A central question in these fundamental biological processes is how dividing cells preserve the memory of gene activation, resulting in epigenetic inheritance. In a recent study, we discovered a new class of non-coding RNAs that we termed SPEARs (S-phase EArly RNAs) which are expressed specifically during DNA replication and help maintain active gene regions.[1] One example that we identified is the oncogene *c-MYC*, whose regulation involves a conserved short RNA sequence, the RM9 motif (Figure 1).[1]

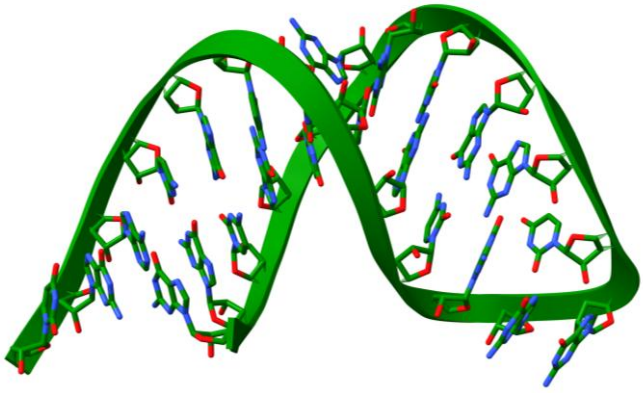

Figure 1: AlphaFold3 prediction of the RM9 motif.[2]

To provide a foundation for understanding how RM9 may contribute to transferring the information of previously activated genes, we aim to analyse its structure by solution-state NMR spectroscopy. We present NOESY-based NMR data that provide initial insights into RM9's conformational flexibility and potential folding behaviour. These findings lay the groundwork for further structural characterisation and analysis of interactions with key regulators of chromatin remodelling such as histone H2A.Z and histone acetyltransferase KAT5, helping to explain how SPEARs modulate *c-MYC* activity and influence epigenetic regulation during the S-phase of the cell cycle.

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Lipocoacervates as a Route Towards Complex Synthetic Cells

Thomas Bissing,[1] Laura Heinen*,[1]

[1] *DWI – Leibniz Institute for Interactive Materials, Aachen, Germany*

Life emerges from the orchestrated interplay and regulation of molecular components within cellular compartments. Various scientific disciplines strive to mimic these processes and to engineer life-like synthetic systems. One of life's key characteristics is compartmentalization, either using membraneless and membrane-bound substructures. Coacervates, for example, form membraneless droplet-like structures spontaneously through associative phase separation of macromolecules. Inside this condensed phase the concentration of specific molecules can be enriched or depleted, while small molecules are still able to permeate the droplets. This dense phase mimics the crowded environment within the cytosol of a living cell.[1] However, the lifetime of such droplets is short due to their propensity to fuse. Unlike coacervates, membrane-bound structures such as liposomes are kinetically stable structures protected by a semi-permeable lipid bilayer, but the lumen is difficult to load with concentrated high-molecular weight contents and functional cell-components.[2]

In this project, we combine the advantages of both types of compartments—coacervates and liposomes—for the bottom-up self-assembly of synthetic cells. The goal is to develop a robust and reliable procedure for the fabrication of lipocoacervates, a hybrid system of coacervate droplets enclosed by a lipid bilayer.

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Synthesis and Characterization of a Novel Thiophene-Functionalized C_{60} Fulleropyrrolidine for Photovoltaic Applications

Cansu Sezgin,[1] İbrahim Erden[1]

[1] *Yıldız Technical University, Department of Chemistry, Istanbul, Turkey*

Fullerenes and their derivatives are among the important functional materials for dye-sensitized solar cells (DSSCs) due to their unique electron affinities, extensive π-conjugation systems and high electron mobilities. Particularly C_{60} fullerene, with its strong electron-accepting character, accepts electrons from photo-excited dye, suppressing back charge transfer at the interface and significantly improving charge separation. It has been clearly demonstrated in the literature that fullerene derivatives serve as electron acceptor in DSSCs, reducing recombination at the TiO_2/dye interface and consequently increasing the open-circuit voltage (V_{oc}).[1,2] Additionally, it has been reported that functionalizing the fullerene structure allows for adjustment of energy levels, which both improves orbital compatibility with the dye and positively impacts device performance.[1]

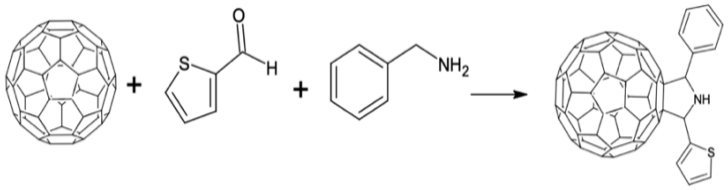

Figure 1: Synthesis of fullerenopyrrolidine using Prato reaction (1,3-dipolar cycloaddition).

The fullerene derivative synthesized in this study is a fulleropyrrolidine structure obtained via a Prato-type cycloaddition reaction on C_{60} fullerene, as shown in Figure 1. This method is based on the addition of an azomethine ylide intermediate to the fullerene double bonds in the presence of an aldehyde and a primary amine, allowing for the controlled integration of functional groups into the structure.[3],[4] The tunability of the energy levels in the post-synthetic fulleropyrrolidine derivatives improves both the orbital overlap with the dye molecule and directly contributes to device performance by optimizing the interaction with TiO_2. Structural characterization of fullurene was determined using FTIR, Q-TOF MS and UV-Vis analysis. In this context, the structure given in the scheme is not only a synthetic example; it also serves as a concrete model of a rational design strategy aimed at improving DSSC performance through a molecular engineering approach.

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Structural characterization of fractionated beech lignin using NMR and ultrahigh resolution mass spectrometry

Wiebke Hadwich[1], Erica Brendler[1], Jan Zuber[1], Martina Bremer[2], Steffen Fischer[2], Carla Vogt[1]

[1] *TU Bergakademie Freiberg, Institute of Analytical Chemistry, Freiberg, Germany*
[2] *TU Dresden, Institute of Plant and Wood Chemistry, Tharandt, Germany*

Lignin has high potential as a renewable resource for aromatic compounds. However, the complex and variable polymeric structure impedes targeted use for chemical production.[1-3] To elucidate the chemical structure of lignin after pulping to pave the way for higher-value applications and more sustainable production of aromatic compounds is the aim of this work. Combining NMR as well as ultrahigh resolution (tandem) mass spectrometry is necessary to shed light to the molecular organization of this highly complex and heterogenous material.

Liquid NMR spectroscopy (^{1}H-, ^{1}H, ^{13}C HSQC-, quantitative ^{13}C-NMR) and solid-state NMR spectroscopy ^{13}C SP/MAS-NMR und CP/MAS-NMR) as well as ultra-high-resolution Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry for solid and soluble samples were combined for the analysis. Beech lignin samples were fractionated with different water/acetone mixtures to separate fragments by polarity.

HSQC-NMR and neutral loss analysis from tandem MS shows that the investigated beech lignin consists predominantly of guaiacyl and syringyl units, which are mainly linked via β-O-4', β-β' and β-5' bonds. Accompanying substances such as sugars, lipids, and tannins were detected in NMR and MS analyses, emphasizing the complexity of the samples. Tandem mass spectrometry was further used to investigate structural differences of characteristic precursor ions in different water/acetone mixtures by correlating the neutral losses after collision induced dissociation.

The combination of NMR spectroscopy and mass spectrometry proved to be complementary and provided consistent results on the structural composition of the beech lignin analyzed. These initial analyses of the molecular organization and linkage patterns represent the first step toward fully realizing lignin's potential as a renewable resource, paving the way for its higher-value applications beyond mere energy production.

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Determination of Amine Content in Polyethyleneimine-Modified Ternary Layered Double Hydroxide

Zehranur Arslan[1], Hüseyin Gündüz[2] , Deniz Gül[2], Tarık Eren[1], Müge Sarı Yılmaz[2]

[1] *Yildiz Technical University, Faculty of Arts and Sciences, Department of Chemistry, Istanbul, Turkiye*

[2] *Yildiz Technical University, Faculty of Chemistry and Metallurgy, Department of Chemical Engineering, Istanbul, Turkiye*

Layered double hydroxides (LDHs) are two-dimensional lamellar materials with positively charged layers and interlayer anions.[1] LDH nanomaterials are evaluated for a wide range of applications including wastewater treatment, energy storage and conversion, CO_2 adsorption, water splitting and even drug delivery.[2] Although LDHs possess adjustable composition and anion-exchangeability, unmodified structures often show limited desired properties due to insufficient functional groups. Trimetallic LDHs have recently gained interest as the incorporation of a third metal ion can overcome key limitations of mono- and bimetallic LDHs, such as weak electronic conductivity, low ion transfer rate, agglomeration, and structural instability. This additional metal also modifies charge density, increases the number of electroactive sites, optimizes the band-gap structure, and enhances electron conduction, leading to superior physicochemical and electrochemical performance.[3] Amine modification is another effective strategy to enhance the functional performance of porous materials. Polyethyleneimine (PEI) provides abundant amine groups, humidity tolerance, and significantly improved CO_2 adsorption capacity, offering synergistic effects when combined with inorganic hosts such as LDHs.[4] In this study, the amine content of polyethyleneimine-modified ternary LDH (PEI-TLDH) was determined. The material was synthesized via co-precipitation method using Mg^{2+}, Al^{3+} and Ca^{2+} cations and functionalized with Polyethyleneimine as amine source. The amine abundance was determined by FTIR analysis and the Hinsberg reagent, in order to evaluate its potential advantages for advanced CO_2 capturing applications.

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Formation of highly selective binding pockets in UiO-type MOFs from pre-connected linkers

Tobias Hennig,[1] Verena Drewes,[1] Erik Rohloff,[1] Andreas M. Schneider,[1] Yasar Krysiak,[1] Sergi Plana-Ruiz,[2] David Heinrich Andrew Bailey,[3] Christian Thoben,[3] Moritz Hitzemann,[3] Stefan Zimmermann,[3] Andreas Schaate[1]

[1] Institute of Inorganic Chemistry, Leibniz University Hannover, Germany
[2] Servei de Recursos Científics i Tècnics, Universitat Rovira i Virgili, Tarragona, Spain
[3] Institute of Electrical Engineering and Measurement Technology, Leibniz University Hannover, Germany

Metal-organic frameworks (MOFs) are a promising class of inorganic-organic hybrid materials, which are characterized by their high intrinsic porosity and their construction from modular building units, which themselves can be functionalized for specific applications. Precise control over such functionalization within MOF pores is highly desired for tailor-made applications, yet hardly realized to date.

Herein we present a novel way to introduce functional groups precisely within a UiO-66 framework, making use of its intrinsic geometry in order to increase affinity towards aliphatic nitro compounds.

For the construction of the framework, we synthesized a dimeric linker[1] featuring two terephthalic acid units bridged by a short urea crosslink (Fig. 1a). A room temperature synthesis using precipitated Zr_6-clusters was adapted.[2] We combined modelling and electron diffraction techniques to determine the arrangement of the urea crosslinks (Fig 1b). When compared to other UiO-66 derivatives, the obtained *pcl*-UiO-66-Urea MOF showed increased affinity towards aliphatic nitro compounds in nitroethane vapor sorption (Fig. 1c).

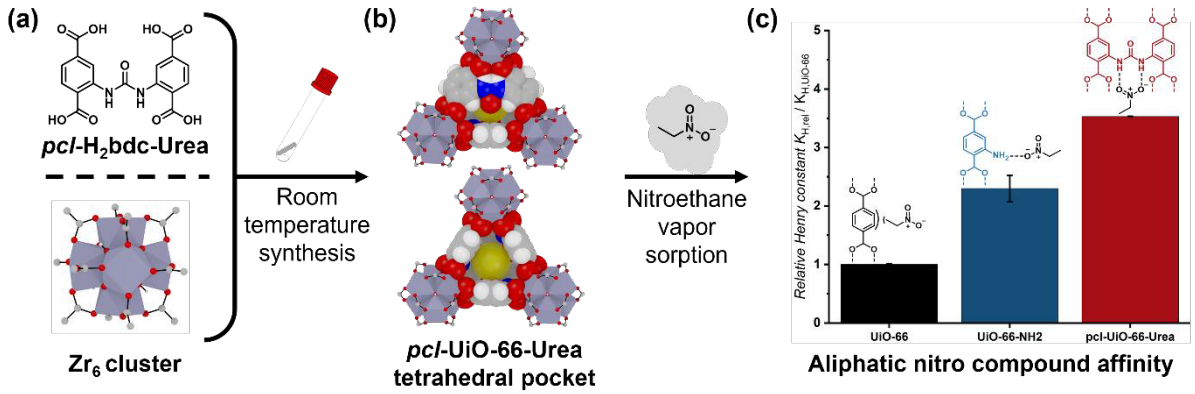

Figure 1: Synthesis, structural characterization and application of *pcl*-UiO-66-Urea MOF. **a)** Room temperature MOF synthesis. **b)** Possible binding pocket linker arrangement. **c)** Nitroethane affinity derived from vapor sorption (298 K) of *pcl*-UiO-66-Urea and reference MOFs with relative Henry constants.

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Exploration of Novel *N*-Difluoromethyl Motifs

Gina Wycich[1] Filip Zivkovic,[1] Jaime Ponce-de-León,[1] Linhao Liu,[1] Franziska Schoenebeck[1]

[1]*RWTH Aachen University, Institute of Organic Chemistry, Aachen, Germany*

The introduction of fluorine atoms is a widely used strategy to tune molecular properties, with more than 20% of all marketed drugs containing fluorine.[1,2] While the trifluoromethyl group has long been valued for its impact on solubility, conformation, lipophilicity, and metabolic stability,[3] the difluoromethyl group has recently emerged as a powerful bioisostere for hydroxy, thiol, and amino groups due to its polarized C–H bond and hydrogen-bonding ability.[4] However, limited synthetic methods have constrained its broader exploration. Given the prevalence of nitrogen in bioactive molecules, new strategies to modify amides and related motifs are highly desirable.[5] We developed methods enabling straightforward access to *N*-difluoromethyl carbamoyl fluorides and *N*-bisfluoromethylated amines. The carbamoyl fluorides serve as versatile building blocks for the synthesis of *N*-difluoromethyl amides, (thio)carbamates, ureas and formamides.[6] Additional installation of a -CF_3 group onto thioformamides enables convenient synthesis of previously inaccessible *N*-(CF_3)(CF_2H) amines via desulfurization-fluorination.[7] Both *N*-fluoromethyl motifs were examined regarding lipophilicity, rotational barriers, and hydrogen bonding and demonstrate high robustness in post-functionalization. Notably, *N*-(CF_3)(CF_2H) amines show enhanced hydrolytic stability and additional H-bonding capability, making them compelling alternatives to previously established N-CF_3 amines.[8]

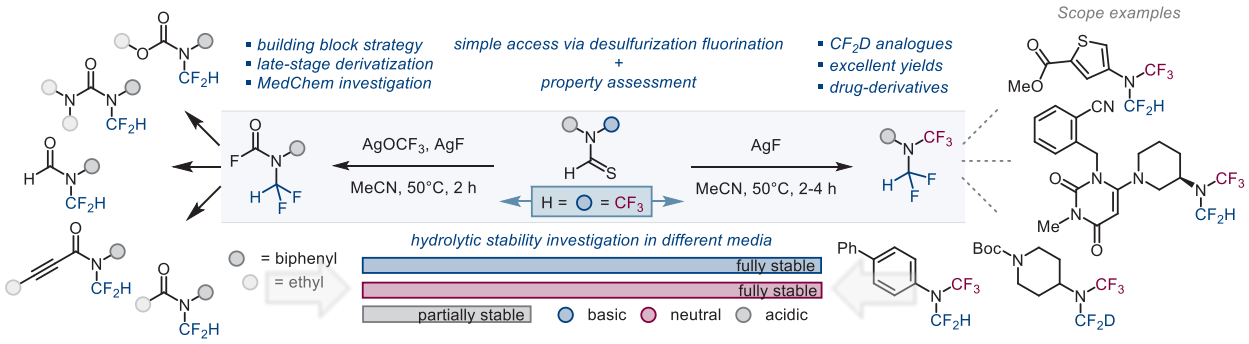

Figure 1: Overview of the developed methodologies.[7,8]

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Abstract FAIR4Chem Award - Supplement Data of Anolytes for All-Iron Redox-Flow Batteries

Marius M. Engler,[1] Michael Stich,[1] Christoph Baumer,[1] Andreas Bund[1]

[1] *Technische Universität Ilmenau, Interdisciplinary Institute for Materials Engineering, Electrochemistry and Electroplating Group, Ilmenau, Germany*

Iron-based redox-flow batteries (Fe-RFBs) have received significant interest as a promising solution for stationary energy storage, owing to their use of cost-effective and environmentally friendly materials. The efficiency and long-term stability are closely linked to the electrochemical properties and material characteristics of the electrodes and electrolytes.[1,2] The electrochemical performance and stability depend strongly on the electrolyte composition. To this end, the fundamental characteristics of various base electrolytes and additives were investigated in this study.[2]

Electrolytes containing iron sulphate or iron chloride were examined regarding their deposition behavior at room temperature. The kinetic data shows a clear advantage in using basic electrolytes consisting of just iron salt and supporting electrolyte with elevated pH (> 2.0). However, further tests show insufficient long-term stability due to the oxidation of Fe^{2+}. An excess (ratio >1:1) of complexing agents / buffers partially inhibits iron deposition to such an extent that various additives and concentration ratios need to be investigated in further studies.[2]

Due to their complexity, providing comprehensive datasets is crucial to ensure the reproducibility and comparability of scientific findings. This paper presents datasets derived from a series of experiments on iron-based half cells electrolytes, including cyclic voltammetry coupled with electrochemical quartz crystal microbalance. It includes detailed information on experimental setups, operating conditions, material properties, and data processing workflows.

Our primary objective is to improve the efficiency of data acquisition and processing while standardizing data preparation and publication in accordance with the FAIR principles. Publishing these datasets increases transparency, supports reproducibility, and fosters collaboration in battery research. In addition, this work served as a pilot project for establishing research data management within our department, providing reusable templates that will reduce future effort. Overall, our commitment to data transparency and standardization promotes scientific progress and advances not only in sustainable energy storage research.

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Bio-based Flame-Retardant Coatings for Enhanced Wood Protection

Damla Cansu Sefa[1], Yakup Atıcı[2], Ebru Ergüven[2], Tarık Eren[1]

[1]Yıldız Technical University, Faculty of Art and Science, Davutpaşa Campus,34220, İstanbul, Türkiye
[2] Kayalar Kimya San. Tic. A.Ş.Tuzla, İstanbul,Türkiye

In recent years, the growing environmental awareness and demand for sustainable alternatives have increased the significance of bio-based materials in flame-retardant research. Among these, *epoxidized soybean oil (ESO)* has received considerable attention as a renewable and versatile polymer precursor due to its accessibility, low cost, and reactive functional groups. These properties make it an excellent candidate for the design of environmentally friendly flame-retardant coatings. [1]. Incorporation of phosphorus-containing compounds, particularly *DOPO (9,10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide)*, can enhance flame retardancy by promoting char formation during combustion and reducing flammability. This strategy offers a promising route for developing halogen-free and sustainable wood protection systems [2].

In this study, two different phosphorus-based molecules were synthesized for potential use as bio-based flame-retardant coatings. The first compound was obtained by modifying epoxidized soybean oil with phosphoric acid (FR-1), while the second was synthesized from DOPO and itaconic acid (FR-2). The chemical structures of the synthesized compounds were characterized by Fourier-transform infrared spectroscopy (FTIR) and nuclear magnetic resonance spectroscopy (^{1}H and ^{31}P NMR). The surface properties of the coated wood samples were evaluated through flexibility, adhesion, Erichsen, hardness, and gloss tests along with small-scale combustion experiments.

Although the flame-retardant tests are still in progress, preliminary findings indicate that the developed bio-based coating systems possess strong potential as effective and environmentally friendly flame retardants for wood protection applications. This work contributes to the ongoing effort toward sustainable and halogen-free flame-retardant materials.

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Non-Equilibrium Statistical Thermodynamics of Motor Proteins in Cells

Leon Jeckel,[1,2,3] Jianshu Cao,[2] Chunte S. Peng[1,2]

[1] *Broad Institute of MIT and Harvard, Cambridge, MA, USA*
[2] *MIT, Department of Chemistry, Cambridge, MA, USA*
[3] *ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland*

In the absence of an unbalanced conformational current J, enzymatic reactions obey Michaelis-Menten kinetics.[1] Such enzymatic systems are Markovian and fluctuate in a non-equilibrium steady-state (NESS).[1,2] Investigating J hence bears implications on the predictability and memory of enzymatic processes.[3,4] In NESS, the fluctuation theorem (FT) relates entropy production to kinetic statistics.[5] It was recently demonstrated how to extend this theory to non-Markovian systems.[6] Experimental measurements of enzyme statistics enable testing for FT violations, and if the case that $J \neq 0$, rate quantification as a function of J and determination of the chemical driving force $\Delta\mu$.[2,6]

Dynein and kinesin are microtubule-based motor proteins which serve as interesting platforms to study statistical single-molecule enzyme kinetics. The two ATP-dependent molecular motors move in 8 nm steps either forwards or backwards. If the associated rates k_+ and k_- are not the same, the FT is violated and $J \neq 0$. Previous analysis of kinesin has suggested that the two rates are very similar, though not identical.[7] For this study, we employ upconverting nanoparticles (UCNPs) as photostable probes in super-resolution microscopy to record motor stepping at nanometer-resolution – a method proven successful in uncovering the dynein motor mechanism.[8] In this work, our goal is to leverage the ability for long-term tracking to determine robust motion statistics. From the waiting time distributions of molecular motor stepping we aim to extract k_+ and k_- with high accuracy and quantify the efficiency of different dynein and kinesin variants based on entropy production.

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Development and Characterization of PAMAM and Starch Based Gels for Slow Release of Urea Fertilizer

Nehir KAYA[1], Aylin KAYMAZ[1], Mustafa Ulvi GÜRBÜZ[1], Metin TULU[1], Tarık EREN[1]

[1] *Yildiz Technical University, Faculty of Art and Science, Chemistry Departmant Istanbul, Turkiye*

Chemical fertilisers are widely used to boost agricultural productivity.[1] One of the most commonly used fertilisers is granular urea, which contains 46% nitrogen. However, due to its low molecular weight and thermal instability, a significant proportion of the nitrogen is lost through volatilisation, leaching and gaseous emissions.[2] Controlled-release fertiliser systems have been developed to overcome these limitations, ensuring more efficient and sustained nitrogen uptake by plants.

Due to its high biodegradability, ease of chemical modification and strong water retention ability in agricultural applications, starch is an attractive natural polymer.[3] PAMAM dendrimers, which are characterised by surface amine groups and internal amide linkages, are widely used in various biological fields and show great promise as a source of nitrogen for agricultural applications.[4]

Within the scope of this study, methacrylate-functionalized PAMAM dendrimers and acrylate-functionalized starch polymers were synthesized. The aim was to obtain urea-loaded, biocompatible, and biodegradable gel systems. Comprehensive characterization studies were conducted on the resulting materials. The release performances of the obtained gels in aqueous media were investigated.

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Multicomponent Rare-Earth Zirconates as New Thermal Barrier Coatings: Reaction behavior at the Al_2O_3 interface

Manuel Schenker,[1] Maren Lepple[1]

[1] *Justus Liebig University, Institute of Inorganic and Analytical Chemistry, Giessen, Germany*

Reducing CO_2 emissions to slow down climate change is one of the biggest scientific challenges in the 21st century. Several options are being studied to reduce the consumption of fossil fuels in the transportation industry. In this context, there is a need to investigate new opportunities to increase the efficiency of aircraft turbine engines and reduce CO_2 emissions. However, complex requirements and further limitations on solutions must be considered, such as the need for lightweight materials. One option to be considered is the optimization of the thermal barrier coating (TBC) in the turbine combustion area, aiming to increase the working temperature and reduce the amount of fuel required.[1]

Yttria-stabilized zirconia (YSZ) has been commonly used as TBC materials in turbines under high temperature exposure. Unfortunately, this standard material has some limitations that need to be overcome, like a phase transition at 1200 °C and the limited corrosion resistance against the harsh environment under working conditions.[2] One of the upcoming alternative materials for TBC applications are the multicomponent zirconates (or also called high-entropy zirconates) with the $RE_2Zr_2O_7$ formula, where the RE site is occupied with at least five rare-earth cations in equimolar proportion.[3]

In the first experiments, these new materials show promising thermophysical properties like high-temperature stability, low thermal conductivity and a matching coefficient of thermal expansion with the underlying metallic substrate. Additionally, this work investigated the behavior at the interface with alumina experimentally by X-ray diffraction, scanning electron microscopy, and energy dispersive X-ray spectroscopy, since alumina is often formed in the interface between the TBC and the metallic components of the turbine. First findings in a bulk mixture of the high-entropy zirconates and alumina show two main reaction products: $REAlO_3$ and $RE_3Al_5O_{12}$. To study the reaction behavior and its kinetics, different conditions in the interface were employed to estimate the lifetime of a TBC system under working application in an airplane turbine. Further investigations are necessary to understand the reaction conditions, estimate opportunities to prevent it, and also to find applicable solutions to use high-entropy zirconates as TBC materials.

Acknowledgement
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Controlled Synthesis and Design of Highly Multiplexed Upconverting Nanoparticles for Live-Cell Imaging

Hyung Jun Kim[1,2#], Alevtina Studenikina[1,2#], Harrison W. Toll[1,2#], Irmuun Tommy Altankhuyag[1,2], Ivana Hsyung[1,2], Kaibo Ma[1,2], João Shida[1,2], Caroline Kim[1,3], Y. Erin Chen[1,3], and Chunte Sam Peng[1,2]

[1]Broad Institute of MIT and Harvard, Cambridge, MA, USA

[2]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, USA

[3]Department of Biology, Massachusetts Institute of Technology, Cambridge, MA, USA

[#]These authors contributed equally.

Optical microscopy has revolutionized our understanding of complex biological systems, providing high-resolution insight into cellular organization and dynamics; however, current fluorescence methods are limited in multiplexing capacity and durability. Simultaneous multicolor imaging using fluorescent dyes is generally restricted to 4 colors.[1] Dyes suffer from photobleaching, hindering unique signals.[2] Unlocking more stable multiplexing would transform our ability to capture the full molecular and spatial complexity of living systems. A new generation of robust, multiplexed optical probes is required.

Upconverting Nanoparticles (UCNPs) exhibit a unique anti-Stokes shift, converting near-infrared excitation into tunable, sharp emissions in the visible region with indefinite photostability and minimal autofluorescence. By changing lanthanide composition, the relative emission intensities can be precisely tuned to create distinct spectral “colors”.[3]

Despite their promise, creating a large library of spectrally distinct UCNPs presents a significant synthetic challenge. UNCPs’ optical properties are highly dependent on nanocrystal size and uniformity, but varying dopant compositions to create different colors alters the nucleation and growth kinetics.[4] This interdependence between composition and morphology presents a significant challenge to produce uniform nanoparticles across a wide multicolor palette. Typical three-step syntheses (ligand exchange, salt addition/drying, and high-temperature growth) require multi-parameter optimization for each individual color.

First, I report a novel, facile method for controlling UCNP synthesis. By precisely tuning the temperature and duration of the second "drying" step, I found that nucleation kinetics could be modulated. This discovery allows me to have a high degree of control of nanoparticle formation while maintaining uniformity. This finding transforms what was previously understood as a passive drying step into a useful control parameter, enabling the facile synthesis of uniform nanoparticles with sizes tunable from 8 nm to 170 nm.

Second, leveraging this new synthetic control, I designed and synthesized a highly multiplexed library of 20 spectrally distinct UCNPs. This method successfully overcomes the kinetic challenges posed by varied dopant compositions. The resulting 20-color palette achieves an average detection accuracy of 97.8%. This work provides both a fundamental advance in $NaYbF_4$ nanocrystal formation and a practical toolkit for enabling highly multiplexed imaging, paving the way for more complex systems-level analyses

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Computational Study of Disease-Associated Variants of Ornithine Transcarbamylase and Double Mutant

Bruno Mochi,[1] Darrin Bath,[1] Mary Jo Ondrechen,[1]

[1] *Northeastern University, Department of Chemistry and Chemical Biology, Boston, USA*

Ornithine transcarbamylase (OTC) deficiency represents the most prevalent urea cycle disorder, affecting approximately 1 in 14,000 to 77,000 live births. This X-linked condition causes toxic ammonia accumulation with devastating neurological consequences; mortality rates exceed 50% in severe neonatal cases. Current treatments, costing $50,000-100,000 annually, merely manage symptoms through dietary restrictions and ammonia scavengers rather than addressing the underlying enzymatic defect. Despite over 500 documented pathogenic mutations, fewer than 20 have been molecularly characterized, creating a critical knowledge gap that impedes therapeutic development.

Our research employs an integrated computational framework to elucidate how mutations disrupt OTC function and identify compensatory strategies for restoring enzymatic activity. We are utilizing quantum mechanics/molecular mechanics (QM/MM) simulations on molecular dynamics snapshots to investigate catalytic mechanisms in wild-type and disease-variant OTC. Our analysis focuses on our identified key active site residues[2], particularly D263, which we hypothesize initiates catalysis through charge donation to ornithine. By examining multiple snapshots from microsecond-scale MD trajectories with high-level QM/MM calculations, we are revealing how specific mutations alter catalytic efficiency at the atomic level.

A compelling aspect of our investigation involves contrasting outcomes of double mutations: Q270R/R40H partially rescues function while K46R/R40H exacerbates dysfunction. Through extensive molecular dynamics simulations combined with Residue Interaction Network (RING) analysis, we are testing whether Q270R stabilizes the C-terminal domain to counteract R40H-induced N-terminal destabilization—a compensatory mechanism absent in K46R/R40H.[3] These findings illuminate how distant residues communicate through protein networks to modulate enzymatic function.

Building on these mechanistic insights, we are computationally screening compensatory mutations for the severe D196Y variant, which reduces ornithine production 50-fold. Preliminary MD studies reveal that Y196 forms aberrant π-π stacking interactions with aromatic residues (W193, W265, F281), preventing essential SMG loop closure. We are evaluating ten rationally designed mutations at positions G197 and N198 to disrupt these pathological interactions while restoring catalytic function. The most promising candidates will undergo experimental validation through site-directed mutagenesis and biochemical characterization.

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Self-Assembly of Cobaloxime on Titanium Dioxide Nanoparticles for Solar Driven Hydrogen Production

Matthew Huebner,[1] Charles Wilson,[1] Phoebe Nitchals,[1] Christine Caputo*[1]

[1] *University of New Hampshire, Department of Chemistry, Durham, United States*

Burning fossil fuels for our increasing energy needs has been shown to contribute to the growing negative effects of climate change.[1] The electrocatalytic and photocatalytic generation of hydrogen from water is of interest as a possible clean and renewable energy replacement for fossil fuels. Hydrogen gas (H_2) is an exceptional candidate for this form of energy storage, and researchers have been extensively exploring electrochemical water splitting methods to produce clean hydrogen gas.[2]

Photocatalysis has been an effective method by reducing hydrogen from water via Ultraviolet irradiation of metal catalysts anchored on semiconductor particles/surfaces.[3] Cobaloxime catalysts are of particular interest due to their simple synthetic preparation, and high catalytic activity for hydrogen generation.[4] We have designed a system where cobaloxime catalyst is anchored to the surface of titanium dioxide (TiO_2) and has been shown to improve electron transfer for photocatalysis.

Here we show the ability for $[Co(dmgH)_2$ (py-4-COOH)Cl] (py-4-COOH = iso-nicotinic acid, dmgH = dimethylglyoxime monoanion) to be prepared by self-assembly on the surface of iso-nicotinic acid functionalized titanium dioxide (TiO_2) nanoparticles when stirred in a solution of methanol. Loading of ISO on the surface of TiO_2 was quantified and compared following treatment of nanoparticles with ISO for different times. Using a loading solution at a concentration of 2.5 mM iso-nicotinic acid (ISO) on TiO_2 resulted in a loading amount of 96.1 nmol ISO/ mg TiO_2 following stirring (2 h) as measured by UV-visible difference spectroscopy. When the cobaloxime catalyst precursor was stirred for 24 h with ISO-functionalized TiO_2 before irradiation, the system produced 0.31±0.11 µmol H_2 compared to 0.31±0.07 µmol H_2 when using the pre-synthesized catalyst. When the cobaloxime catalyst components ($CoCl_2$ and 2 Equiv. dimethylglyoxime ($dmgH_2$)) was stirred for 24 h with ISO-functionalized TiO_2 before irradiation, the system produced 0.15±0.07 µmol H_2.

This shows that the need to synthesize $[Co(dmgH)(dmgH_2)$(py-p-COOH)Cl] in advance is unnecessary, and avoiding this step is more economical in terms of time and materials needed. This process of loading the TiO_2 with the anchored pyridyl ligand attached to the surface beforehand has not been previously explored and it could lead to improvements in development of this and other catalytic systems.

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Electrochemiluminescence of Pt Complexes in Organic Media utilising Co-reactants

Caroline Witter,[1] Damian Antonio Pedraza Daza,[2] Gabriela Marzari,[2] Leon Geerkens,[1] María Victoria Cappellari,[1] Cristian A. Strassert,[1] Fernando Fungo[2]

[1] *University of Münster, Institute of Inorganic and Analytical Chemistry, 48149 Münster, Germany*

[2] *Universidad Nacional de Río Cuarto, Facultad de Ciencias Exactas, Físico-Químicas y Naturales, Río Cuarto, Argentina*

Electrochemiluminescence (ECL) can be described as the generation of light by the utilisation of electrochemical techniques. Due to its low background emission, it is a sensitive method often employed in immunoassays. While most of the current applications are based on $[Ru(bpy)_3]^{2+}$ or $[Ir(ppy)_3]$ as well-established luminophores, ongoing efforts are made to develop new metal complexes with electrochemiluminescent properties.[1,2]

This work explores the potential application of newly designed Pt complexes as ECL luminophores. Their suitability was tested together with various co-reactants in acetonitrile as organic medium. The photophysical and electrochemical characterization is complemented by measurements of pulsed techniques and ECL spectra.

A colourful glow for future improvements!

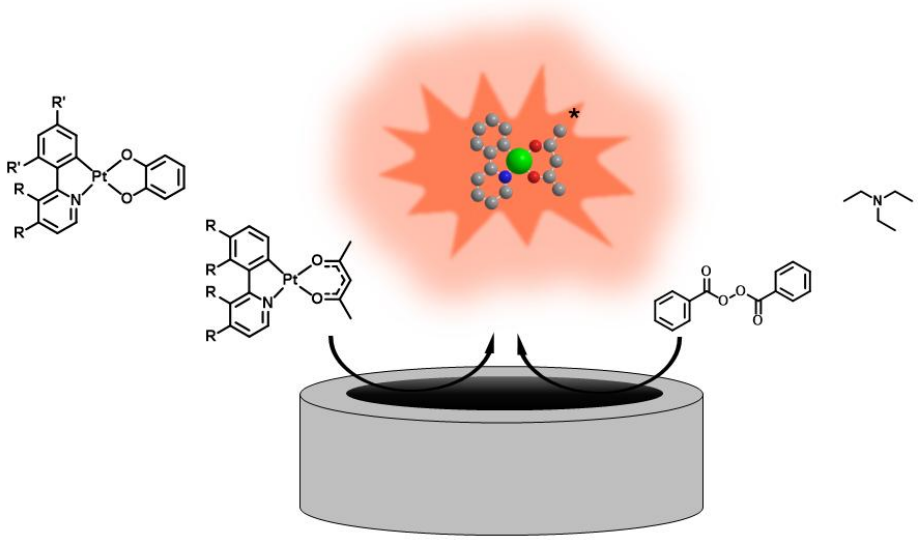

Figure 1: Working principle of the ECL with co-reactants and investigated complexes.

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Dual-functional adamantane-substituted phthalocyanine: a crosslinker and photosensitizer for PDT-active nanogels

Enfal Civril,[1] Burak Yıldız,[2] Aysun Değirmenci,[1] Rana Sanyal,[1] M. Kasım Şener,[3] Amitav Sanyal,[1]

[1] *Bogazici University, Department of Chemistry, 34342 Bebek, İstanbul, Türkiye*
[2] *Ege University, Program of Refinery and Petrochemical Technology, 35800 Aliağa, İzmir, Türkiye*
[3] *Yıldız Technical University, Department of Chemistry, 34210 Esenler, İstanbul, Türkiye*

Conventional cancer treatment approaches, including chemotherapy, radiotherapy, and surgery, are often limited by systemic toxicity, the development of drug resistance, and tumor recurrence. As a minimally invasive alternative, photodynamic therapy (PDT) has gained increasing attention. PDT operates through the interaction of light, molecular oxygen, and a photosensitizer (PS) to generate cytotoxic reactive oxygen species (ROS), predominantly singlet oxygen ($^1O_2$). Among various photosensitizers, phthalocyanine-based compounds have emerged as highly effective PDT agents due to their strong absorption in the near-infrared region, high singlet oxygen quantum yields, and superior photostability, enabling efficient and localized cancer cell eradication upon light activation.[1-3]

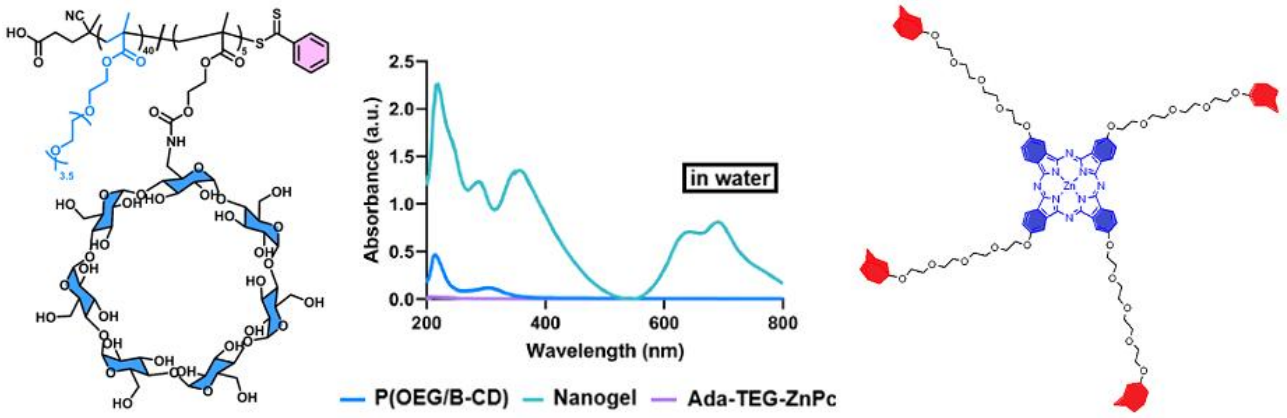

Figure 1: Chemical structures of **Ada-TEG-ZnPc**, **P(OEG/*β*-CD)** and UV-Vis absorption spectra of the nanogel and its precursors.

In this study, an adamantane-substituted phthalocyanine (**Ada-TEG-ZnPc**) was synthesized and employed in the preparation of nanogels via host–guest interactions with cyclodextrin-functionalized hydrophilic polymers (**P(OEG/*β*-CD)**) (Fig. 1). The PDT activity of the resulting nanogels was systematically investigated. Furthermore, the available cyclodextrin cavities on the polymer backbone were utilized for post-functionalization with adamantane-substituted cell-penetrating peptide, enabling the fabrication of targeted nanogels with enhanced cellular specificity.[4]

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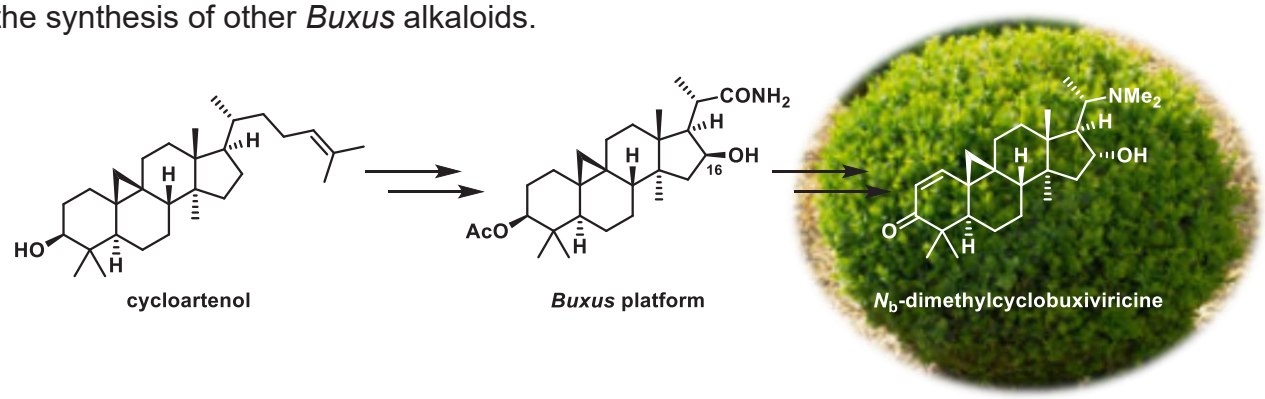
Synthetic efforts toward N_b-dimethylcyclobuxiviricine and other *Buxus* alkaloids

David Gleisberg,[1] Prof. Dr. Philipp Heretsch[1]

[1] *Leibniz University, Institute of Organic Chemistry, Hannover, Germany*

To date, more than 200 steroidal alkaloids from plants of the *Buxus* genus have been isolated and identified. Apart from their complex chemical structure, many of these *Buxus* alkaloids exhibit potent biological activities such as cytotoxic, anticholinesterase or cardiovascular activities. Despite this, the class of *Buxus* alkaloids is strongly underrepresented in the field of natural product synthesis.

The steroidal alkaloid N_b-dimethylcyclobuxiviricine is known for its anticancer activity, which is attributed to its degrading effect on the mutant p53 gene.[1] Due to its promising anticancer activities, this alkaloid serves as the first target for exploration of the synthetic space of *Buxus* alkaloids. Given the similar steroidal skeleton, a semisynthetic approach was chosen, starting from readily available cycloartenol. As a first critical step, a method for the selective C–H-oxidation at the C-16 position was established.[2] Further modifications of the oxidation state led to a γ-lactone, that could be opened by aminolysis. The resulting amide could serve as a starting point for incorporating the characteristic amine moiety into the steroidal side chain by Hofmann degradation. Furthermore, the amide could serve as a strategic platform for the synthesis of other *Buxus* alkaloids.



Scheme 1: Synthesis towards N_b-dimethylcyclobuxiviricine starting from cycloartenol.

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Vibronic coupling and energy transfer in HRP

B. Ali,[1] M. Hinterthan,[1] L.J.G.W. van Wilderen,[1] J. Bredenbeck[1]

[1] *Goethe University, Institute of Biophysics, Frankfurt (Main), Germany*

Everybody has heard of hemoglobin, the red blood cells responsible for transferring oxygen through our bodies. That transport is possible due to the iron atom in the center of the protein which binds the oxygen molecule and thus carries it through the bloodstream. Hemoglobin belongs to a group of proteins called “heme-proteins”, which include cytochrome C, myoglobin and horseradish peroxidase (HRP). All these proteins contain the heme chromophore in their catalytic site and perform different vital functions, e.g. storage and enzymatic functions. With the recently developed 2D-VE (two dimensional vibrational electronic) spectroscopy, the vibronic coupling and energy transfer processes around protein chromophores can be investigated.[1] This includes the interactions between the heme and its surrounding molecules. Due to commercial availability and its ability to bind to small molecules, HRP was chosen for the study. To better understand the environment of the heme and how the molecules bind to it, small molecules, such as CO[2–5], are introduced to HRP and modulate the spectral properties. It coordinates to the ferric center of heme and forms ternary complexes with benzhydroxamic acid (BHA)[5] and its derivatives.[2,4] While the UV-spectra show no differences with the small molecules binding to the protein, the IR-spectra show respective shifts and eliminations of the CO-bands.

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Molecular Analysis of Active Pharmaceutical Ingredients by Liquid Chromatography High-Resolution Mass Spectrometry

Jonathan Andreas,[1] Helly Johanna Hansen,[1] Christopher Paul Rüger[1]

[1] *University of Rostock, Department Life, Light and Matter, Rostock, Germany*

Plant extracts contain a multitude of substances of pharmacological and medical interest, with Traditional Chinese Medicine (TCM) especially utilizing them for the treatment of a wide range of illnesses.[1] However, the characterization and quantification of ingredients contained within these extracts pose a unique challenge for analytics, due to their complex molecular structure, as well as mixtures and isomers further complicating accurate, replicable measurements.

For this purpose, a microwave-assisted methanol extraction method[2] was modified for the dried root of *Paeonia lactiflora* (*Paeoniae Radix Alba*), which is a commonly cited extract in TCM. Part of the crude extract was then purified by liquid-liquid-extraction. All resulting extracts were analyzed by establishing and optimizing a high-resolution LC-ESI-MS method with total ion mobility spectroscopy (TIMS) as a means of adding a structural dimension and resolving shape and size of the ionized compounds. Early screenings were conducted by direct infusion (DI) TIMS-MS measurements, followed by coupling with a HPLC-DAD system.

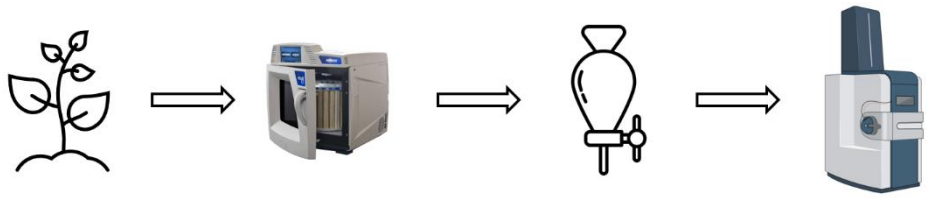

Figure 1: Extraction and Analytics workflow.

DI-MS measurements confirmed the presence of the isomers albiflorin and paeoniflorin, two pharmaceutically active ingredients known for their anti-inflammatory and antioxidative effects.[3] Other terpene glycosides could also be identified, with literature suggesting substances like benzoyl- or galloylpaeoniflorin.[4] Separation of certain compounds, like benzoylpaeoniflorin, could be observed in the different extracts. Further method improvement promises reliable characterization of pharmaceutical compounds from natural sources.

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P100

Chiral Azo-based Calamitic Liquid Crystals with Tailored Mesomorphic and Photoresponsive Behaviour

Gürkan Karanlık,[1] Barış Sezgin,[2] Ceren Can Karanlık[1]

[1] *Yildiz Technical University, Department of Chemistry, Davutpaşa Campus, 34220, Esenler, Istanbul, Turkey*

[2] *Süleyman Demirel University, Department of Chemistry, 32260, Cunur, Isparta, Turkey*

Liquid crystals (LCs), which exist in a mesomorphic state and tend to adopt ordered arrangements while maintaining fluidity, are such sensitive functional materials that their mesomorphic behaviour can drastically change even in minor alterations in the molecular architecture. By carefully fine-tuning the structural parameters such as the type of central cores, linking groups or terminal chains, the mesophase characteristics of LCs can be precisely controlled, resulting in a wide range of advanced applications.[1,2]

Chiral liquid crystals (CLCs) have an important place in both fundamental science and modern technology due to extraordinary characteristics that result from their lack of mirror symmetry. The introduction of a chiral segment into the molecular structure can lead to the formation of helical structures which reveal chiral mesophases such as chiral smectic C (SmC*) and chiral nematic (N*) phases showing selective light reflection, ferroelectric, antiferroelectric and fast electro-optic response behaviours. For this reason, chiral liquid crystal materials have been used in high-performance displays, photonic devices, optical filters and light-modulation technologies.[3,4]

In this work, we report the synthesis, characterization, mesomorphic and photoresponsive investigations of a series of azo-functionalized chiral liquid crystals comprising three aromatic rings terminated with a fixed branched chiral chain at one side and *n*-alkyl chains with varying lengths at other end. The structures of the mesogens were clarified by NMR (^{1}H- and ^{13}C-NMR) and mass spectroscopic techiniques and mesomorphic behaviours were explored by polarized optical microscopy (POM) and differential scanning calorimetry (DSC). The results showed that the length of the terminal chains has significant effect on the mesomorphic temperature intervals and the presence of a chiral unit resulted in chiral mesophases which are very important for advanced (opto)electronic devices.

This work has been supported by Yildiz Technical University Scientific Research Projects Coordination Unit. Project Number: FKD-2025-7389.

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Biased ligand activation of the receptor tyrosine kinase FGFR1c studied in living cells

Annabelle Brauel[1], Marina S. Dietz[1], Julian Kompa[2], Kai Johnsson[2] & Mike Heilemann[2]

[1] *Institute of Physical and Theoretical Chemistry, Goethe University Frankfurt, Frankfurt am Main, Germany*

[2] *Department of Chemical Biology, Max Planck Institute for Medical Research, Heidelberg, Germany*

Receptor tyrosine kinases (RTKs) regulate essential cellular processes such as proliferation and differentiation and are activated through ligand-induced dimerization and autophosphorylation.[1–3] A single RTK can interact with multiple ligands, which may differentially modulate downstream signaling pathways, a phenomenon known as ligand bias.[2,4] The fibroblast growth factor receptor FGFR1c is a splice variant of FGFR1, one of the four receptors within the FGFR family, that responds to a range of fibroblast growth factors (FGFs) and plays an important role in development and disease.[2] The activation strength of these different ligands, as well as the kinetics of receptor activation in living cells, are unknown.

In this project, we measure the temporal dynamics of FGFR1c activation for different FGF ligands in living cells using single-particle tracking (SPT). FGFR1c was fused to a HaloTag7 self-labeling protein tag, transiently expressed in CHO-K1 cells, and labeled with fluorophore-conjugated HaloTag7 ligands.[5] Ligand-specific temporal response profiles of FGFR1c were captured by either sequential imaging or long-term SPT,[6,7] and show distinct kinetic patterns and activation strengths in single living cells.

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Synthesis Of Flame Retardants From Cashew Nut Shell Waste And Their Use in Polyurethane Foam Production

Büşra Paçaman,[1] Yusuf YİVLİK,[2] Prof. Dr. Tarık Eren[1]

[1] *Yıldız Technical University, Faculty of Art and Science, Chemistry Department Istanbul, Turkiye*

[2] *Flokser Chemical Industry and Trade Joint Stock Company Istanbul, Turkiye*

Bio-based flame retardants have gained increasing attention as sustainable alternatives to petroleum-based and halogen-containing additives, which are associated with environmental and health concerns.[1] Cardanol, a phenolic lipid derived from cashew nut shell liquid (CNSL), is an abundant biomass waste and a versatile precursor for functional materials, and transforming cashew nut shell waste into high-performance functional chemicals offers a compelling dual benefit of waste valorization and potential improvements in fire safety.[2] Here, a phosphorus-containing cardanol derivative was synthesized via reaction with dichlorophenylphosphine oxide, characterized by NMR and FTIR, and incorporated into rigid polyurethane foam formulations. The modified foams exhibited increased char yield and improved flame-retardant performance in LOI and UL-94 tests, consistent with phosphorus-driven condensed-phase mechanisms reported in the literature.[3–5] Mechanical properties such as density, dimensional stability, and compression strength remained within acceptable ranges, demonstrating that cardanol-based flame retardants can enhance fire performance without compromising structural integrity. This work highlights the potential of CNSL-derived phosphorus additives as industrially viable, environmentally friendly flame-retardant solutions for polyurethane foams.

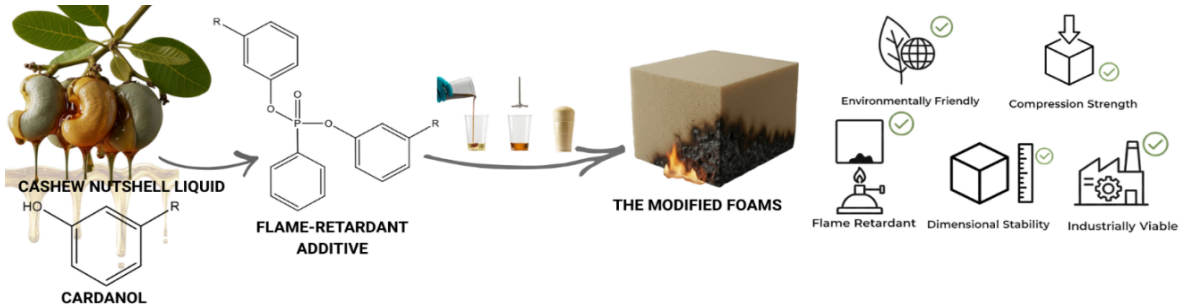

Figure 1: Schematic illustration of the synthesis of a phosphorus-containing cardanol-based flame retardant and the properties of the resulting rigid polyurethane foams.

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Investigation of a Potential Relation between the Metallophores Rhodopetrobactin B and Methylolanthanin in *M. extorquens* PA1

Hannah Goerlach,[1] Sandro Sperzel,[1] Sophie M. Gutenthaler-Tietze,[1] Michael Mertens,[1] Lena J. Daumann.[1]

[1] *Chair of Bioinorganic Chemistry, Heinrich Heine University Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany*

Lanthanides (Lns) are increasingly important in modern technologies and also essential for the metabolism of some methylotrophic bacteria.[1–3] Despite this relevance, the molecular details of how bacteria acquire Lns are still under investigation. Recently, methylolanthanin (MLL) was identified as a potential metallophore for Lns (=lanthanophore) in *Methylorubrum extorquens* AM1, resembling the known siderophore rhodopetrobactin B (RPB B).[4] The related bacterial strain *M. extorquens* PA1 produces both MLL and RPB B, providing an opportunity to explore a possible biosynthetic or functional link between these two chelators. This is of interest because MLL does not seem to meet the classic expectations for being a lanthanophore, e.g. it precipitates with Lns in test tube conditions, instead of solubilizing them.[5] Motivated by the close structural resemblance between RPB B and MLL, we herein investigated a potential relation between MLL and RPB B. To this end, we synthesized ^{13}C-labeled RPB B, and conducted feeding experiments with *M. extorquens* PA1, followed by analysis of the bacterial supernatant for ^{13}C-labeled MLL by LC-HRMS. Both MLL and RPB B were quantified, revealing nanomolar concentrations of MLL, as compared to RPB B in micromolar concentrations and an influence of the growth medium on the production of both metallophores. With our investigations, we are contribute to the understanding of the lanthanide(III) and iron(III) uptake machinery in methylotrophic bacteria.

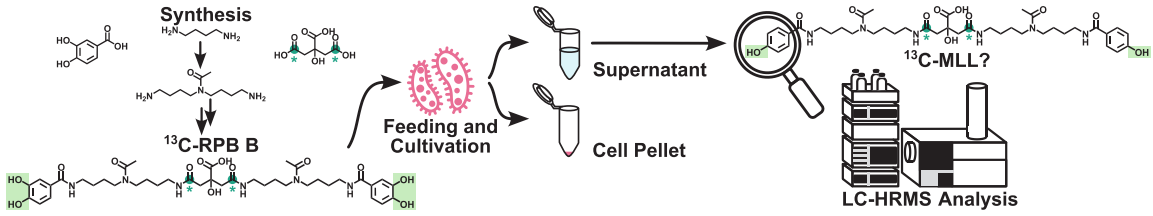

Figure 1: Schematic illustration of the synthesis of ^{13}C-labeled rhodopetrobactin B, feeding experiments with *M. extorquens* PA1 and analysis of the bacterial supernatant by high resolution mass spectrometry with regards to the potential formation ^{13}C-labeled methylolanthanin.

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Direct Mechanocatalysis – A novel technique for sustainable Catalysis

Maximilian Wohlgemuth,[1] Maike Mayer,[1] Lars Borchardt[1]

[1] *Ruhr-University Bochum, Inorganic Chemistry, Bochum, Germany*

The concept of direct mechanocatalysis is a novel concept of catalysis neither utilizing light, thermal heating nor electric potential as in conventional catalysis, but simply mechanical energy. In this mechanochemical approach the use of milling materials made from metals such as Pd, Ni, or Cu are both, catalyst, and energy transmitter and thus the addition of catalyst powder or advanced ligand system becomes obsolete. However, its scalability has been limited due to the cost of catalytically active metals and the wear of milling tools. Due to this issue we developed an electroplating concept, where simple steel materials were electroplated with the needed active catalyst metal.[1]

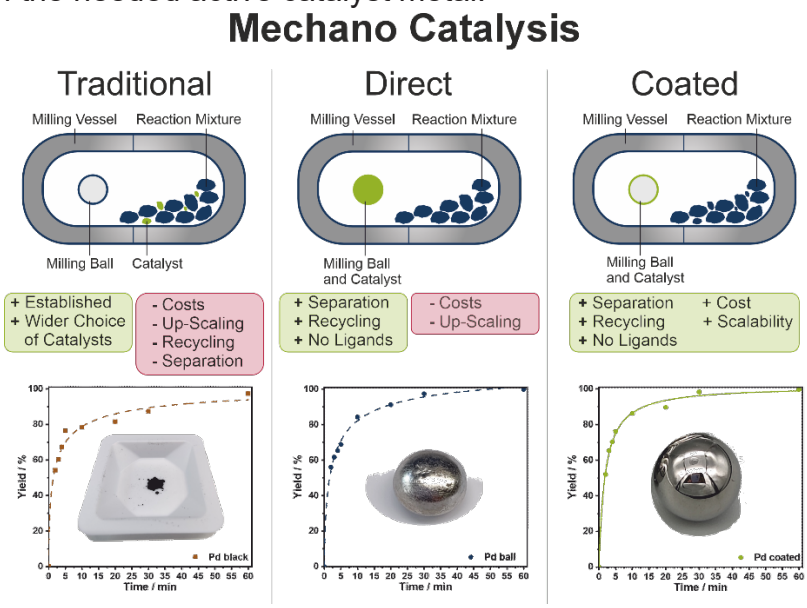

Figure 1: Efficiency of different mechanocatalyitical concepts for the Suzuki reaction.

We first showcase this concept for a type of reactions that is commonly in the hand of homogeneous catalysis – C-C-cross coupling reactions catalysed by Pd and Cu. We show how various, even sterically-demanding and deactivated reagents, can be converted quantitatively in as little as 60 minutes via Suzuki-, Sonogashira-, Heck-, or Glaser coupling. We further advance this concept to the selective oxidation of alcohols to aldehydes using gold-coated milling balls.[2] Finally we show how even hydrogenation reactions can be conducted via this approach using milling vessels that are internally coated with Pd, Ru, Ni.[3] By translating this technique to reactive extrusion we were able to bring direct mechanocatalysis to large scale applications.[4]

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Amino-Acid functionalized polyelectrolytes for stimuli-responsive biomedical applications

Lena M. Lipka[1], Christian Jahns [1], Jonas De Breuck [1], Meike N. Leiske[1,2]

[1] *University of Bayreuth, Macromolecular Chemistry, Bayreuth, Germany*
[2] *Bavarian Polymer Institute, Bayreuth, Germany*

Polyelectrolytes represent a versatile platform for the design of biocompatible and stimuli-responsive materials, which remain a major challenge in medical applications. Their solubility and solution behavior are strongly influenced by electrostatic repulsion along the polymer backbone as well as environmental parameters such as solvent, pH, salt concentration and temperature, largely dependent of whether the polymers are polycationic, polyanionic or mixed systems.[1] In this work, polymers based on acrylamides are synthesized *via* a straightforward one-step reversible addition–fragmentation chain-transfer (RAFT) polymerization and subsequently functionalized through post-polymerization modification with bio-based amino acids (cf. Figure 1). This strategy enables the creation of a versatile library of anionic and zwitterionic polyelectrolytes with tunable charge character and chain mobility.

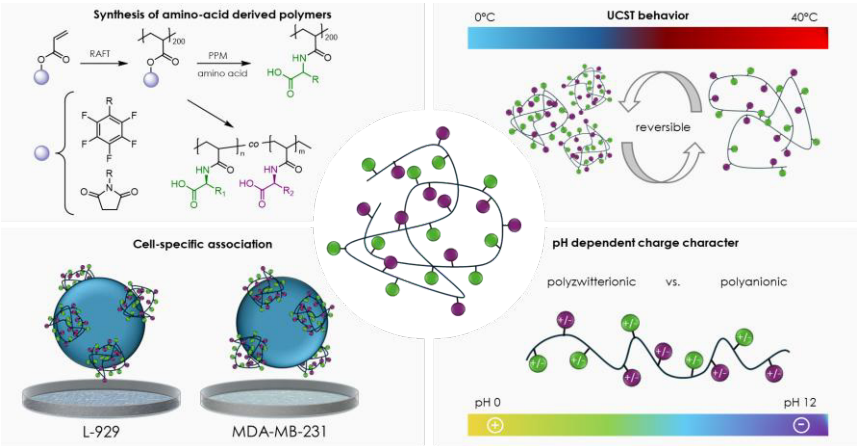

Figure 1:Synthesis and investigation of polyelectrolytes based on polyacrylates with amino-acid derived sidechain modifications.

The resulting polymers are systematically investigated with respect to their thermal and pH-responsive behavior, complex formation and structure–property relationships, highlighting correlations between amino-acid structure, charge distribution and polymer dynamics. Furthermore, interactions with biological systems are evaluated using cell assays with MDA-MB-231 and L929 cells to assess biocompatibility and cell-specific association.[2] Overall, these results provide insight into the application potential of amino-acid-functionalized polyelectrolytes for biomedical uses such as drug delivery systems.

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When Thulium Turns Two: Intense & Colourful Emissions

Moritz J. Dango,[1] Claudia Wickleder*[1]

[1] *University of Siegen, Inorganic chemistry group, Siegen, Germany*

The alkaline earth bromides MBr_2 (M = Mg, Ca, Sr, Ba) exhibit excellent optical properties when doped with a small percentage of divalent thulium ions. They exhibit up to three emission bands simultaneously. The energetic position of the emission maxima is strongly dependent on the crystallographic environment.[1] Depending on the compound, emission colours ranging from blue and green to red and infrared are feasible.[2] Due to the very low stability of Tm^{2+} compared to other divalent rare earths such as Eu^{2+} or Yb^{2+} and the resulting challenging synthesis of the doped compounds,[3] very little is known about the luminescence of Tm^{2+}-doped systems.

The unique electronic structure of Tm^{2+} ions also allow the doped compounds to be used as efficient upconversion materials.[4] This is otherwise only possible with trivalent rare earths and their parity-forbidden, narrow-band f-f transitions. The broad and tuneable emission bands based on parity-allowed transitions of Tm^{2+} have many advantages over conventional trivalent systems. These novel materials have a wide range of potential applications, such as LED materials or security phosphors for banknotes. The upconversion properties open up additional fields of application, such as bioimaging, drug release processes, telecommunications, and improvement of solar cell efficiencies.

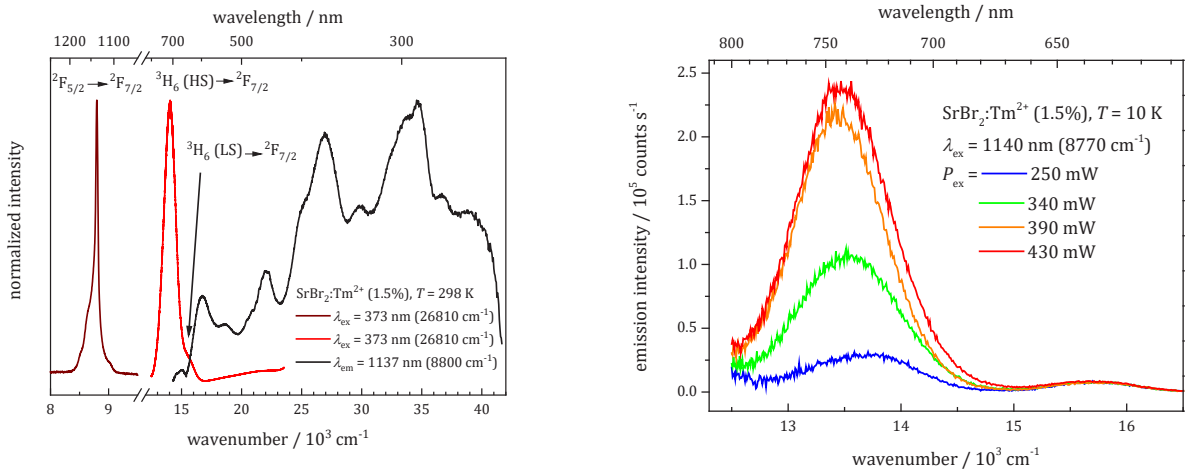

Figure 1: Room temperature emission and excitation spectrum of $SrBr_2:Tm^{2+}$ (left) and upconversion emission spectra of $SrBr_2:Tm^{2+}$ at 10 K (right).

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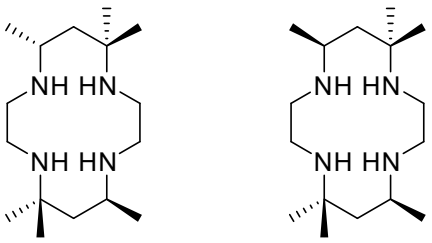
Macrocyclic iron complexes and their reactivity toward various oxidizing agents

Kevin Keller, Prof. Dr. Siegfried Schindler

Institute of Inorganic and Analytical Chemistry,
Heinrich-Buff-Ring 19, 35392 Gießen, Germany

Oxygenation reactions play an important role in the chemical industry. Every year, large quantities of products are manufactured through such processes. For example, adipic acid is obtained through several steps from the oxygenation of cyclohexane. From a sustainability perspective, most of the industrial syntheses are far from ideal. To develop more sustainable methods, modelling the active site of metallo enzymes, which carry out oxidation reactions via reactive oxygen intermediates, is promising. These intermediates often involve iron–oxo species. Nam, Que[1] and co-workers, as well as Schaub[2] et al., have succeeded in synthesizing mononuclear iron–oxo species using strong oxidants such as e.g. ozone together with the TMC (1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane) ligand. More recently, Ray[3] and co-workers demonstrated with cyclam complexes that this can also be achieved using cyclam and molecular oxygen as the oxidant. This raises the question of how other cyclam derivatives behave under similar conditions, particularly when they are chiral. Since our research group has previously gained experience using tet a/b as ligands in oxygen activation with copper, this project presents the corresponding results obtained from experiments on the analogous iron complexes.[4]



tet a tet b

Figure 1: Molecular structure of rac-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane (tet a and tet b)

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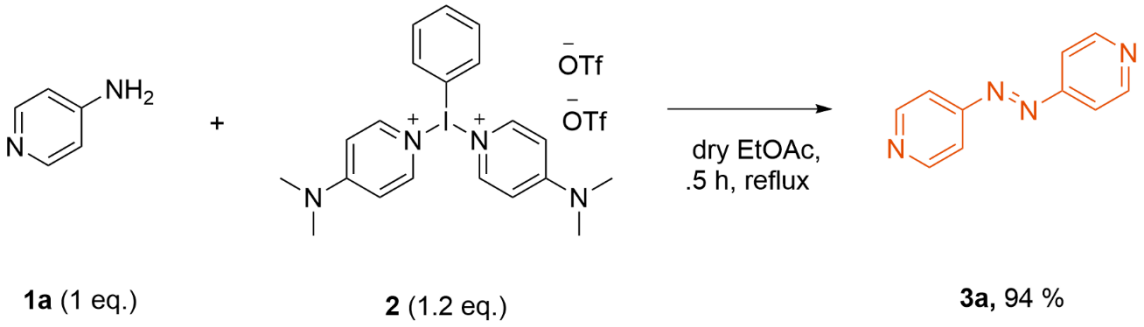
Hypervalent-Iodine-Mediated Oxidative Coupling: A High-Yielding Route to Functionalized Azopyridines and Azobenzenes

Raj Kumar Samanta, Elric Engelage, Robert Weiss*, Stefan M. Huber*

Ruhr University Bochum, Bochum, Germany

A metal-free oxidative coupling of substituted aminopyridines as well as aromatic amines using a hypervalent-iodine reagent **2**, affording excellent yields under mild conditions, is described. [1,2] The presented method is attractive regarding short reaction time, operational simplicity, scalability and high functional group tolerance.

Aromatic azo compounds are classic examples of colourful chemistry because their -N=N- group acts as a strong chromophore that gives them their intense colour. In this study, next to their synthesis, we investigate a small library of azopyridines and azobenzenes to explore how molecular structure governs colour as well as photophysical and electrochemical behaviour. We e.g. evaluate the acid-base responsiveness of **3a** using a strong acid such as triflic acid, followed by reversal deprotonation with triethylamine.



1a (1 eq.) **2** (1.2 eq.) **3a,** 94 %

Scheme 1: Synthesis of 4,4'-azopyridine using a hypervalent-iodine reagent

We also evaluated the different solvent effects, primarily through the $n \rightarrow \pi^*$ transition of **3a**. The absorption spectra remained well defined in different solvents and showed a clear, systematic solvatochromic response. A polar protic solvent like water showed blue shift while the nonpolar solvent showed red shift.

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Injectable photocurable hydroxyapatite-polyester composites for bone repair

Nina Wojniak,[1] Ita Dąbkowska,[1] Amna Sadiq,[1] Agata Goszczyńska,[1] Mirosława El Fray[1]

[1] *West Pomeranian University of Technology in Szczecin, Department of Polymer and Biomaterials Science, Faculty of Chemical Technology and Engineering, Szczecin, Poland*

Bone fractures are among the most common injuries requiring surgical intervention. They are typically stabilized using implantable fixation devices, such as plates and wires, most often made from titanium alloys. However, this approach is invasive and may require a second procedure for implant removal, which increases the risk of complications. Consequently, there is a growing demand for minimally invasive, injectable biomaterials that cure *in situ* and support bone regeneration. In this context, biodegradable, photocurable polymers offer an attractive platform for injectable, *in situ* curing systems.[1]

In pursuit of a biocompatible and bioactive biomaterial, attention was directed toward hydroxyapatite (HAP)-containing polymer composites. A promising route was identified using plant-derived building blocks, including biomass-derived 2,5-furandicarboxylic acid (FDCA) and dilinoleic diol (DLD) obtained from vegetable oils.[2] These building blocks were used to prepare photocurable polyester macromonomers as the organic matrix for HAP-filled composites.

A prepolymer (macromonomer) was synthesized from FDCA and DLD *via* zinc acetate-catalyzed esterification and subsequently functionalized with methacryloyl chloride to introduce photocrosslinkable methacrylate end groups. Hydroxyapatite was then incorporated into the methacrylated macromonomer at six loadings (10-60 wt%), and the formulations were crosslinked under UV irradiation (λ = 365 nm) in the presence of a photoinitiator (Omnirad 2022).

The chemical structure of the methacrylated macromonomer was confirmed by nuclear magnetic resonance (NMR) spectroscopy. The hydroxyapatite-filled composites were characterized by Fourier transform infrared (FTIR) spectroscopy, and their morphology was examined by scanning electron microscopy (SEM). The influence of hydroxyapatite loading on selected properties relevant to biomedical use, including bioactivity, was evaluated to identify compositions with the most favorable balance of processability and performance.

Acknowledgements: This work has been supported by research project Preludium Bis4 from the Polish National Science Center „New composite biomaterials prepared by photocrosslinking”, UMO-2022/47/O/ST5/01653

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Catalytic Selective C–N Bond Metathesis of Tertiary Alkyl Amines

D. T. Egger,[1] C. Zachau,[1,#] E. Studer,[1,#] S. Makai,[1,2,#] S. Kotesova,[1] H. Park,[3] Z. Lian,[2] H. Zhong,[1] T.-L. Choi,[3] B. Morandi [1,2,*]

[1] *ETH Zürich, D-CHAB, Laboratorium für Organische Chemie, Zürich, Switzerland*
[2] *Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany*
[3] *ETH Zürich, D-MATL, Laboratory for Polymer Chemistry, Zürich, Switzerland*
[#] *denotes equal contribution*

Reversible cleavage and re-formation of C–N bonds in tertiary amines would be a powerful strategy for chemical synthesis, given their ubiquity in bioactive molecules.[1] A metathesis approach for tertiary amines remains underexplored, in part because exchange at a trivalent nitrogen can rapidly produce complex combinatorial product mixtures.[2–4] Here we present an iridium-catalyzed single-bond metathesis of tertiary alkyl amines under mild conditions as part of our ongoing interest in catalytic carbon–heteroatom single-bond metathesis reactions.[5,6] We show that careful choice of substituents provides practical selectivity handles, enabling selective cross-metathesis between tertiary amines for the late-stage modification of *N*-heterocycles and synthesis of bioactive scaffolds, including pharmaceutically relevant motifs. Furthermore, we demonstrate the potential of this methodology for step-growth synthesis of polyamine polymers. Finally, we harness the predictable combinatorial complexity of statistically distributed product mixtures and apply our system to molecular data storage.

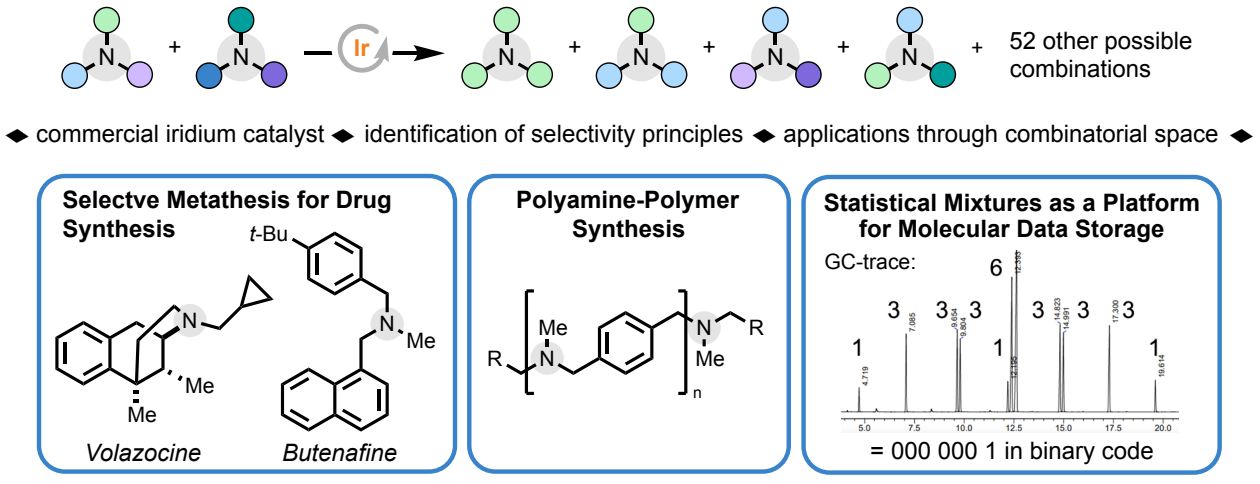

Figure 1: Iridium-catalyzed metathesis reaction of tertiary alkyl amines and applications to organic synthesis, polymer synthesis, and molecular data storage.

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P111

Phenanthrenequinone-based Organic Cathode for the Use in Rechargeable Magnesium Batteries

Noushine Dorrani,[1] Hendrik Koger,[2] Daniel B. Werz,[1] Ingo Krossing,[2]

[1] *University of Freiburg, Institute for Organic Chemistry, Freiburg, Germany*
[2] *University of Freiburg, Institute for Analytical and Inorganic Chemistry, Freiburg, Germany*

The need to replace lithium in chemical storage systems is imminent. Novel battery systems with multivalent anodes like magnesium, calcium or aluminium are more and more investigated but they lack suitable and competitive cathode materials.[1] Organic-based cathodes have been of interest for more than two decades. Their advantageous properties allowed by the versatility of the possible redox-active molecules, combined by their synthesis from refinery waste make organic cathodes to promising alternatives to transition metal oxides-based cathodes. However, the solubility of the organic active material in the electrolyte leading to a capacity decay, combined with the low potentials leave room for improvement in the field of organic/multivalent-batteries.[2–4]

This work focuses on phenanthrenequinone-based polymers as high-voltage cathode for the use in magnesium batteries, supported by a fluorinated weakly coordinating aluminate-based electrolyte. The formation of a *chelate* complex with magnesium ions upon discharge allows to reach a high voltage of up to 3.5 V *vs*. Mg^{2+}/Mg, combined with a high theoretical capacity of 230 mAh/g.

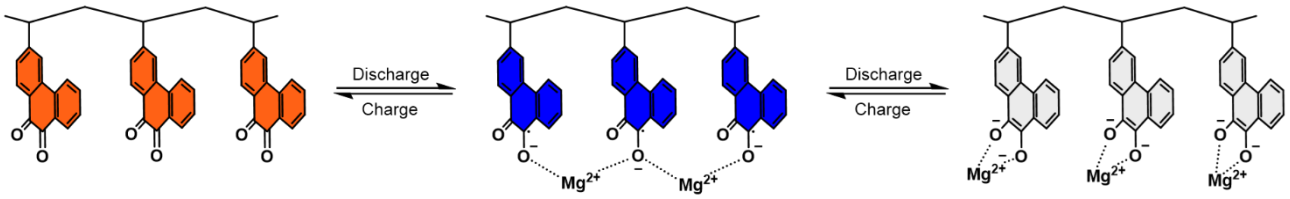

Figure 1: Schematic representation of magnesium intercalation and quinone-reduction at the cathode upon discharging.

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Efficient Visible-Light Photocatalytic Dye Degradation by Novel Mn(II)-Based Cyclotriphosphazene Coordination Polymers

Yunus Zorlu,[1] Rabia Emir,[1] Elif Özcan[1]

[1] Gebze Technical University, Department of Chemistry, 41400, Gebze, Kocaeli, Türkiye

yzorlu@gtu.edu.tr

The persistent contamination of aquatic environments by organic dyes, notably methylene blue (MB) and rhodamine B (RhB), highlights an urgent need for sustainable, visible-light-driven photocatalysts. In this study, three novel Mn(II)-based coordination polymers (PCP-27, PCP-28, and PCP-29) were solvothermally synthesized using a cyclotriphosphazene-derived tetracarboxylate ligand combined with divergent N-donor ancillary ligands (2,2'-bipyridine, terpyridine, and phenanthroline). Single-crystal X-ray diffraction revealed that these ancillary ligands direct the assembly of 1D motifs into robust 2D supramolecular networks via π-π stacking and hydrogen bonding, with PCP-29 demonstrating superior thermal stability up to 370 °C. Optical characterization confirmed narrow band gaps (1.98–2.45 eV), enabling high photocatalytic activity under visible light. Notably, PCP-29 achieved over 90% degradation of MB and RhB within 90 minutes. Mechanistic investigations, supported by electrochemical impedance spectroscopy and radical scavenging experiments, established that the choice of auxiliary ligand critically dictates the electronic structure and the dominant reactive species (OH for PCP-27, PCP-28 and PCP-29). PCP-29 high activity, coupled with its excellent reusability, underscores the effectiveness of cyclotriphosphazene scaffolds in designing robust, recyclable, and visible-light-driven photocatalysts for environmental applications.

This study was supported by the Scientific and Technological Research Council of Türkiye (TÜBİTAK) under Grant No. 122Z456. Additionally, Y.Z. acknowledges the financial support from the Turkish Academy of Sciences (TÜBA) Outstanding Young Scientists Award Program (TÜBA-GEBİP).

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Investigation of the Behavior of Biomass-Based Carbon Quantum Dots as Corrosion Inhibitors on Steel Surfaces and in Acidic Environments

Damla ZORCU, [1] Seden Beyhan[1]

[1] *Istanbul Technical University, Faculty of Science and Letters, Istanbul, Turkey*

Due to their easy synthesis, low cost, and non-toxic structure, CQDs have attracted significant attention in recent years as environmentally friendly inhibitor candidates in corrosion protection applications.[1] In this study, the inhibitory effect of carbon quantum dots (CQDs) synthesized from bay leaves by hydrothermal method on the corrosion behavior of carbon steel in 1 M HCl medium was investigated. CQDs obtained as a result of hydrothermal treatment lasting 24 hours at 225 °C can effectively interact with the metal surface thanks to their nano-sized structures and surface functional groups.

The corrosion behavior was evaluated with 24-hour weight loss experiments; the corrosion rate was calculated from the obtained metal loss values. The corrosion rate was expressed in mm/year, taking into account the surface area and metal density of the amount of material removed from the metal surface per unit time. In the solution without CQDs, the weight loss for carbon steel was determined as 0.622 g and the corrosion rate as 72.27 mm/year. With increasing CQD concentration, a significant decrease in these values was observed due to the formation of a more stable and compact protective layer on the steel surface. The highest inhibitory effect was obtained at a CQD concentration of 1000 mg/L; under this condition, weight loss decreased to 0.0068 g, corrosion rate to 0.79 mm/year, and an inhibition efficiency of 98.21% was achieved.

Electrochemical analyses supported the inhibitory mechanism based on surface interactions of CQDs. The shift in open circuit potential from −423.5 mV to −404.2 mV and the increase in polarization resistance from 3.11 to 4.68 Ω·cm² in 1 M HCl medium containing 500 mg/L CQD revealed that CQDs made the metal surface more passive through adsorption and limited charge transfer. The fluorescence properties and functional surface structures of CQDs play a decisive role in the formation of this adsorption-based protective layer.

Consequently, bay leaf-derived carbon quantum dots, thanks to their environmentally friendly structure and strong surface interaction properties, can be considered an effective corrosion inhibitor for carbon steel in acidic environments and offer a promising alternative for sustainable metal protection strategies.

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Ligandfree reductive amination *via* Pd-coated mechanocatalysis

Lars Beißel,[1] Maximilian Wohlgemuth,[1] Lars Borhardt[1]

[1] *Ruhr-University Bochum, Inorganic Chemistry, Bochum, Germany*

Reductive amination is one of the most used reactions in the synthesis of pharmaceuticals and fine chemicals. Solution-based reductive amination often needs stochiometric amounts of reducing agents like boron hydrides which can lead to toxic side products. Molecular H_2 is a more sustainable reducing agent, while in solution the reaction needs external heating, high pressures, and complex catalyst systems. Here we present a catalytic approach, by using the concept of direct mechanocatalysis with gas mechanochemistry, which already was used for simple hydrogenation reactions.[1] For this we used Palladium coated milling vessels as catalyst with polypropylene milling balls at ambient H_2 pressures (5 bar). While higher milling frequencies for the whole reaction time led to formation of the alcohol, low frequencies did not lead to the amine formation. Therefore, a reaction protocol with two different milling frequencies was developed. The simple option to program the change of mill frequency from 25 Hz to 35 Hz after 1 h during the reaction enabled a one-pot synthesis without interruption of the reaction. This reaction protocol led to high yields of 70 % to 95 % for the reaction between benzaldehyde and primary amines and 14 % to 21 % for secondary amines. For corresponding hydrochloride salts similar yield were observed which allows reductive amination with normally gaseous amines without the handling of highly corrosive and toxic gases i.e., in the case of methyl and ethyl amine. The reaction between aniline aromatic aldehydes yielded 72 % to 92 %, while aliphatic aldehydes yielded up to 43 % yield. The usage of ketones led to yields between 13 % and 31 %, respectively.[2]
Compared to the reaction with sodium borohydride only slightly lower yield were observed, while the formation of side products was avoided and lowering the toxicity of the reaction.
The usage of rather soft bulk material also led to constant yield over five reactions which shows that this low abrasion procedure can be used to perform the synthesis of fine chemicals.

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Halogen-substituted terpyridine-benzimidazole derivatives as dual-mode optical sensors of pressure and temperature

Fang Zhao[1], Christian Hernández-Álvarez[1], Illia E. Serdiuk[2], Michał Mońka[2], Sebastian Mahlik[2], Marcin Runowski[1]

[1] *Adam Mickiewicz University, Faculty of Chemistry, Poznań, Poland*

[2] *Institute of Experimental Physics, Faculty of Mathematics, Physics and Informatics, University of Gdansk, Gdansk, Poland*

Designing molecular systems with controllable luminescence responses to external stimuli is essential for the development of high-performance optical sensors.[1,2] Herein, two halogen-substituted terpyridine-benzimidazole derivatives (Br-TBI and I-TBI) were synthesized, and their luminescence responses to pressure and temperature were systematically investigated under UV excitation. The emission intensities of both compounds are strongly influenced by oxygen concentration, enabling their application as optical vacuum-pressure sensors. Under low-pressure conditions, suppressed oxygen-induced quenching leads to enhanced luminescence sensitivity, whereas at higher pressures the quenching effect gradually saturates, resulting in a modulated optical response. Meanwhile, both compounds exhibit well-defined temperature-dependent luminescence variations, allowing temperature sensing within the investigated range. Notably, halogen substitution induces distinct photophysical behaviors, leading to different pressure- and temperature-dependent sensing characteristics.

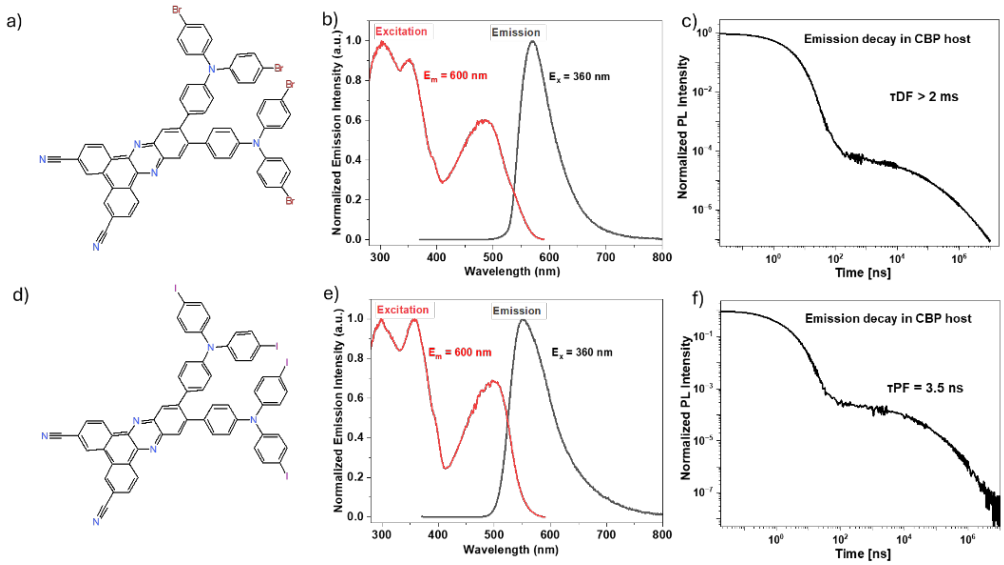

Figure 1: Structural formulas of the synthesized organic compounds, i.e. Br-TBI (a) and I-TBI (d); excitation (red curves) and emission (black curves) spectra (b,e) and fluorescence decay profiles (c,f) of the Br-TBI (b,c) and I-TBI (e,f) derivatives.

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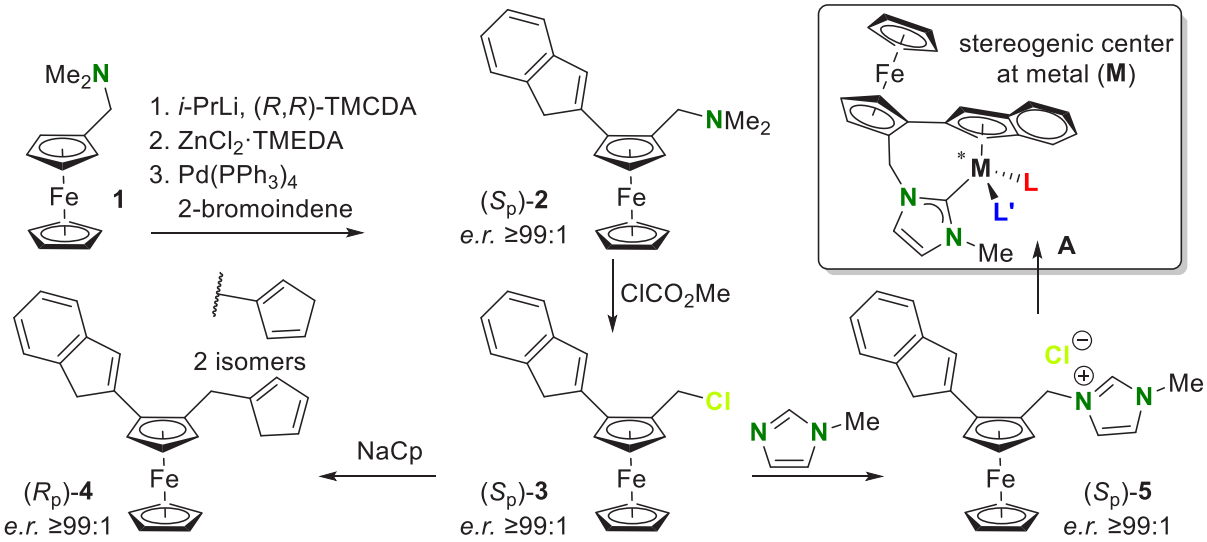
Planar Chiral Ferrocene Ligands for Bridged Ansa(-Half) Sandwich Metallocenes with Stereogenic Metal

Sasha Conrad,[1] Paul-Erik Schneider,[1] Carsten Strohmann[1]

[1]*TU Dortmund University, Department of Inorganic Chemistry, Dortmund, Germany*

Planar chiral ferrocenes are often used as a chiral backbone for ligands in asymmetric catalysis.[1] However, synthetic strategies for such ligands usually require stoichiometric amounts of chiral auxiliaries and labor-intensive synthesis routes, particularly when special functional groups are needed for the final ferrocene product.[2] This leads us to the challenge of providing facile access to planar chiral ferrocenes for asymmetric ligands. We faced this challenge by enantioselective *ortho*-lithiation of achiral **1**. The reaction led to *e.r.* up to ≥99:1 and was also feasible with catalytic amounts of (*R*,*R*)-TMCDA.[3] We utilized this enantiomerically pure lithium aggregate for the enantioselective *ortho*-functionalization by Negishi coupling to introduce an indene ligand to form (S_p)-**2** in a single step. Previously, this transformation required a six-step synthesis route reported by Anderson *et al.*[4]



Scheme 1: Overview of the discussed synthetic procedures

With this facile access in hand, we utilized the reactive key compound (S_p)-**3** to form the ligands [(R_p)-**4** and (S_p)-**5**]. These ligands are expected to direct the configuration of the stereogenic center at the metal diastereoselectively (**A**). This control could be advantageous in catalytic processes where a stereogenic transition metal center forms as an intermediate.

References:

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Tunable BODIPY-Containing Water-Soluble Polymers for Antimicrobial Photodynamic Therapy: Synthesis and Performance

Jannik Fryn,[1] Tony Le Gall,[2] Franck Thétiot,[3] Tristan Montier,[2] Gilles Lemercier,[4] Ulrich Jonas [1]

[1] *University of Siegen, Macromolecular Chemistry, Siegen, Germany*
[2] *Université de Bretagne Occidentale, INSERM, UMR 1078, Brest, France*
[3] *Université de Bretagne Occidentale, CEMCA, UMR 6521, Brest, France*
[4] *Univ. Paris Cité, ITODYS, UMR 7086, Paris / Univ. Reims Champagne-Ardenne, France*

Antimicrobial resistance represents a critical global health threat, necessitating the development of novel therapeutic strategies.[1] Antimicrobial photodynamic therapy (aPDT), a spatially targeted approach utilizing light and photosensitizers to generate reactive oxygen species (ROS), offers a promising alternative to conventional antibiotics. However, most photosensitizers exhibit poor solubility in aqueous or biological media, limiting their bioavailability and clinical translation.[2] To overcome this challenge, we report the synthesis and evaluation of a novel series of boron-dipyrromethene (BODIPY)-containing polymers for potential biomedical applications against different Gram-positive or Gram-negative strains. As model strains *Staphylococcus aureus* and *Pseudomonas aeruginosa* were chosen. The polymers were designed to incorporate multiple comonomers to achieve water solubility, biocompatibility, and tuneable hydrophobicity for enhanced efficacy. *In vitro* assays demonstrated efficient ROS generation, low cytotoxicity, and notable antibacterial activity against both bacterial species regardless of antibiotic resistance profile. These findings highlight the potential of these polymers as a platform for targeted aPDT, offering a promising strategy to combat antibiotic resistance.

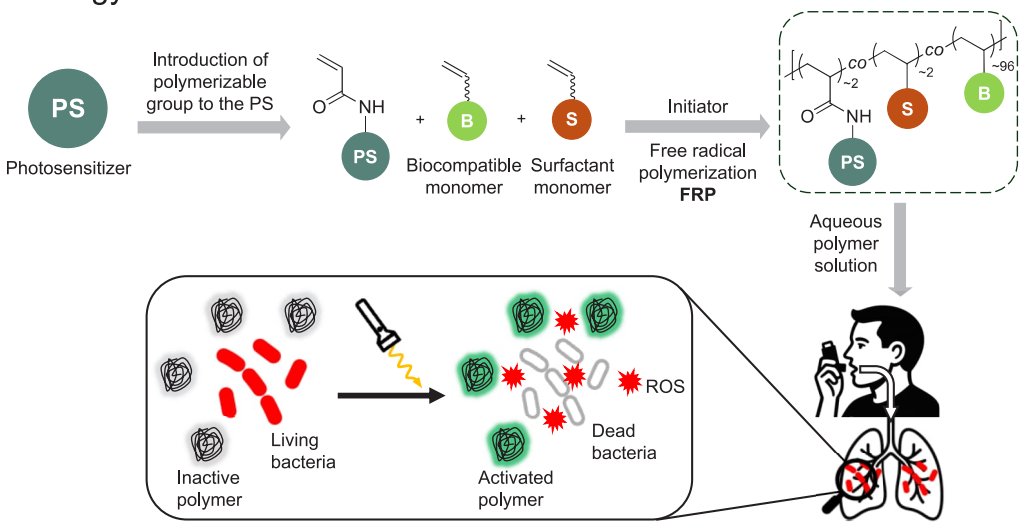

Figure 1: General project scheme with aPDT polymer synthesis (top), exemplary application (bottom right), and mode of action (bottom left).

References:

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Catalytic asymmetric enolate alkylation of carbonyl compounds with polyfunctional Lewis acid/onium salt catalysts

Johanna Haußmann[1], Alexander Beck,[2] Dominik Hornung,[1] Michael Mistele,[1] Alexander Allgaier,[3] Wolfgang Frey,[1] Joris van Slageren,[3] Johannes Kästner[2] and René Peters[1]

[1] *University of Stuttgart, Institute of Organic Chemistry, Stuttgart, Germany*
[2] *University of Stuttgart, Institute for Theoretical Chemistry, Stuttgart, Germany*
[3] *University of Stuttgart, Institute for Physical Chemistry, Stuttgart, Germany*

Direct enolate alkylation is a fundamental method in organic synthesis. Asymmetric versions of the reaction enable the construction of α-stereogenic structures prevalent in pharmaceuticals and natural products. However, existing catalytic asymmetric approaches are often limited by substrate scope and practical applicability, often depending on less efficient auxiliary-based strategies.[1] To overcome these challenges in asymmetric α-alkylation, a Lewis acid/imidazolium salt catalyst has been developed for the alkylation of β-ketoesters.

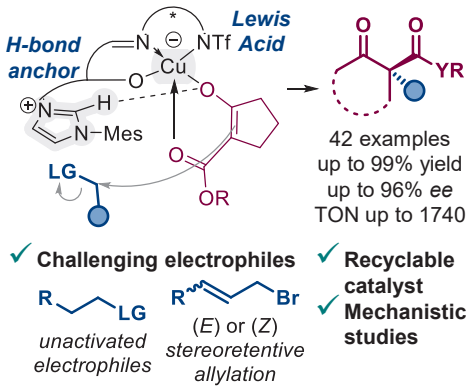

Figure 1: Catalytic asymmetric enolate alkylation of carbonyl compounds with imidazolium-based Cu(II)-complex.

This catalyst is readily synthesized in four simple steps from commercially available starting materials, offering both robustness and air stability. Reactions proceed efficiently under atmospheric conditions, providing high product yields. A detailed mechanistic investigation, including control experiments, kinetic studies, microkinetic modeling, and DFT calculations, was conducted to elucidate the catalyst's mode of action. The method's versatility was demonstrated through successful reactions with a wide range of carbonyl substrates and alkylating agents.

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Accelerated discovery of energy transfer catalyzed dearomative cycloadditions through a data-driven three-layer screening strategy[1]

Debanjan Rana,[1] Carla Hümpel,[1] Ranjini Laskar,[1] Leon Schlosser,[1] Subhabrata Dutta,[1] Constantin G. Daniliuc,[1] Frank Glorius[1]*

[1] *University of Münster, Institute of Organic Chemistry, Münster, Germany*

Dearomative cycloaddition of (hetero)arenes through visible-light-mediated energy transfer (EnT) has emerged as a powerful strategy for the construction of complex three-dimensional frameworks with high medicinal relevance in a straightforward manner. However, EnT-catalyzed intermolecular cycloadditions are mostly limited to bicyclic (hetero)arenes, while monocyclic (hetero)arenes remain underexplored owning to their high triplet energy barriers. The discovery of new reactivity involving potential heteroarene substrates undergoing energy transfer catalyzed dearomative cycloadditions, either experimentally or computationally, represents a major challenge due to the broadness of the chemical space. Thus, a predictive tool for obtaining excited state properties, such as the triplet energy, would guide substrate selection and improve the experimental success.

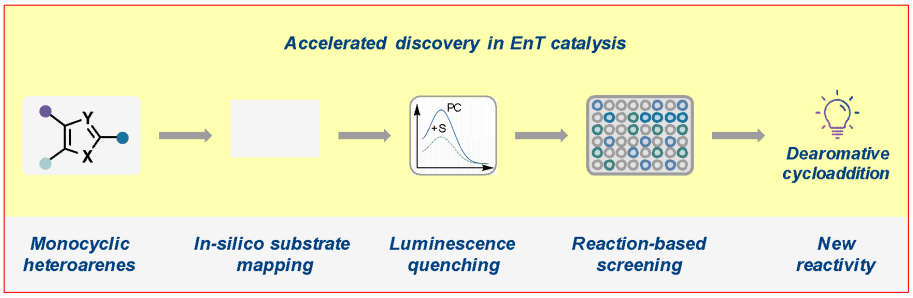

Figure 1: Three-layer screening strategy for accelerated discovery in EnT catalysis.

In this work, we present a three-layer screening strategy, combining data science tools for predicting excited-state properties,[2] luminescence quenching studies and reaction-based screening, towards the accelerated discovery of novel structure-reactivity relationships of monocyclic (hetero)arenes. Employing this data-driven protocol, we discovered the EnT-catalyzed dearomative cycloaddition of thiophenes as well as azoles with alkenes/ bicyclo[1.1.0]butanes, accessing C(sp^3)-rich 3D motifs. We envision this synergy of machine learning and reaction screening methods to function as a versatile platform for accelerated reaction discovery in energy transfer photocatalysis.

References:

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Young Chemists Network (JCF) Marburg

Dilan Gillary Arulnesan,[1] Malwine Lühder,[1] Luca Schipplick[1]

[1] *Philipps University of Marburg, Young Chemists Network, Marburg, Germany*

The Young Chemists Network (JCF) Marburg is a diverse group of approximately 15 active students from bachelor's, master's, teacher training and doctoral programs (Fig. 1A) who are committed to voluntary work in the field of chemistry on behalf of the German Chemical Society (GDCh).

At the Department of Chemistry at Philipps University of Marburg, JCF Marburg regularly organizes events for students and staff. A central element is the annual Chemistry Department Day (Fig. 1B), which provides all research groups with a platform to present their work and promotes both scientific and personal exchange. In addition, JCF Marburg regularly invites external speakers from academia and industry. These lectures are complemented by follow-up discussions, offering space for in-depth exchange, questions and direct interaction with the speakers (Fig. 1C). Furthermore, JCF Marburg organizes site visits and industrial tours (Fig. 1D), which provide insights into non-academic career paths and strengthen contacts with the chemical industry.

As part of a nationwide and international network, JCF Marburg is also active beyond the local level. In 2023, JCF Marburg jointly organized the Spring Symposium (FJS) together with JCF Frankfurt and JCF Gießen in the neighboring city of Gießen.



Figure 1: A) Team of the Young Chemists Network (JCF) Marburg. B) Chemistry Department Day at the Department of Chemistry, Philipps University of Marburg. C) Invited lecture by Prof. Dr. Amitabh Banerji (University of Potsdam) followed by a discussion session. D) Group photo taken during an industrial site visit at CSL Behring.

Determination of Elemental Content in Raspberry Plant Parts and Associated Soil

Jelena Mrmošanin,[1] Stefan Petrović,[1] Denis Mitov,[1] Katarina Milenković,[1] Ana Radosavljević,[1] Aleksandra Pavlović,[1] Snežana Tošić,[1]

[1] *University of Niš, Faculty of Sciences and Mathematics, Niš, Serbia*

Raspberry (*Rubus idaeus* L.) occupies an important place in Serbian fruit production.[1] The quality of the fruit and its safety for human consumption largely depend on soil properties. In this study, the content of 20 elements was determined in different raspberry tissues (root, shoot, leaf, and ripe and unripe fruit) and associated soil from plantations of different ages (28 and 2 years old) using inductively coupled plasma optical emission spectrometry (ICP-OES). Plant and soil samples were prepared by wet digestion on a hot plate.[2] The prepared samples were analysed using the external calibration method.

In the soil of both plantations, the order of macroelements was Mg > Ca > K > P > Na. The content of Na is over 100x lower than the content of other macroelements. In the root, shoot, ripe and unripe fruit of both orchards, the contents followed the order: K > Ca > P > Mg > Na, while in the leaf the order was: K > Ca > Mg > P > Na. During the ripening of the fruit, concentrations of macroelements generally decrease except for Na. The order of concentrations of essential microelements in the soil of both plantations is as follows: Fe > Zn > Cr > Cu > B. The concentrations of Fe, Zn and Cr in the soil are higher in the new plantation, while the concentrations of Cu and B are higher in the old plantation. In the plant tissue, Fe was the most abundant essential microelement, with the highest concentration in the root while the content of Cr is the lowest. In the fruit, the content of Fe increases during ripening, the content of B and Zn decreases, the content of Cu increases slightly, while the content of Cr varies the least. Of the probably essential elements in the soil, Mn predominates. The new orchard contains higher levels of Mn, Ni, and Co, while Ba and Si are more abundant in the old orchard. In all plant tissues, the order was: Mn > Ba > Si > Ni > Co. Manganese is particularly accumulated in the leaves of the old orchard. Toxic and potentially toxic elements in the soil followed the order: Al ≫ Pb > Cd. In the root, shoot and leaf, the order is: Al > Pb > Cd. As a rule, the values are higher in the old plantation except for Pb in the roots. In the fruit, the order was Pb > Al > Cd, with all contents higher in ripe fruit. Mercury and arsenic were not detected in any sample.

The distribution of the analyzed elements among raspberry plant parts is consistent with data reported in the literature, while differences in absolute values and variations between individual plantations can be explained by differences in agroecological conditions.[3]

References:

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Electrochemical and spectrophotometric evaluation of antioxidant activity in *Rosa agrestis* Savi fruits

Katarina Milenković,[1] Jelena Mrmošanin,[1] Denis Mitov,[1] Stefan Petrović,[1] Ivana Rašić Mišić, Emilija Pecev-Marinković,[1] Aleksandra Pavlović[1]

[1] *University of Niš, Faculty of Sciences and Mathematics, Department of Chemistry, Niš, Serbia*

Cyclic voltammetry (CV) measurements were performed using a glassy carbon electrode at different scan rates (25, 50, and 75 mV s^{-1}) and pH values (2.0, 4.5, and 7.0). Based on the anodic current intensity and voltammetric response, the optimal conditions were established at a scan rate of 75 mV s^{-1} and pH 4.5. The effect of the scan rate on the anodic current intensity at pH 4.5 is presented in Figure 1.

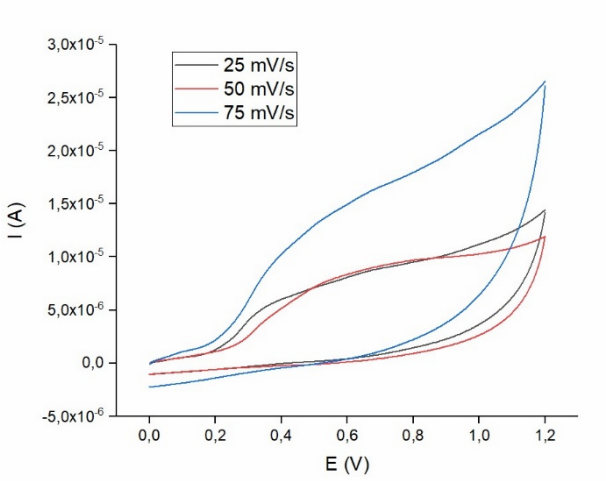

Figure 1: Optimization of scan rate at pH 4.5

Cyclic voltammograms recorded in the potential range from 0 to 1200 mV exhibited characteristic anodic peaks. The first anodic peak appeared in the range from 0.467 to 0.510 V, while the second was observed between 0.724 and 0.778 V; both peaks can be attributed to the oxidation of catechin-type flavonoids.[1] This indicates the presence of phenolic compounds in the extracts that are electrochemically active within the investigated potential range. In parallel with the electrochemical analysis, total phenolic content (TP), total flavonoid content (TF), vitamin C content, and antioxidant activity were determined using ABTS, DPPH, CUPRAC, and FRAP assays. TP values ranged from 76 to 116 mg GAE g^{-1} dry weight (DW), while TF values varied between 41 and 58 mg CE g^{-1} DW. Vitamin C content ranged from 11.48 to 12.7 mg g^{-1} DW. Antioxidant activity values were 219–289 mg TE g^{-1} DW (ABTS), 84–107 mg TE g^{-1} DW (DPPH), 290–394 mg TE g^{-1} DW (CUPRAC), and 0.64–1.26 mmol FE g^{-1} DW (FRAP). Based on the obtained results, a pronounced antioxidant potential of *Rosa agrestis* Savi fruits was confirmed, along with good agreement between electrochemical and spectrophotometric methods. Also, CV could be an alternative to spectrophotometric methods to determine antioxidant activity.[2]

References:

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Trends in Pentafluoroorthotellurate-based Silanes

Friederike Oesten,[1] Prof. Dr. Sebastian Riedel[1]

[1] *Freie Universität Berlin, Institut für Chemie und Biochemie, Berlin, Germany*

Among the few silicon compounds containing the pentafluoroorthotellurate group ($OTeF_5$, teflate) that have been reported, $Me_3SiOTeF_5$ is the only one that has been fully characterised.[1] In contrast, $Si(OTeF_5)_4$ was only briefly mentioned in the literature and its characterization is limited to its melting point.[2] Therefore, we investigated the substitution of chlorides in different organosilicon chlorides with teflate groups towards silicon compounds with an increasing teflate content.

Inspired by the synthesis of $Me_3SiOTeF_5$, several other $R_3SiOTeF_5$ (R = alkyl, aryl) compounds could be obtained by reacting $HOTeF_5$ or the easier to handle $AgOTeF_5$ and the corresponding R_3SiCl. Based on these results, synthetic routes for $R_2Si(OTeF_5)_2$ (R°=°Me, Et, ^{i}Pr, Ph) and $RSi(OTeF_5)_3$ (R = Me, Et, ^{t}Bu, Ph) species were developed. Currently we are adapting the synthesis to the corresponding germanes $R_xGe(OTeF_5)_{4-x}$ (x = 3–0, R = aryl, alkyl) and have already been able to make $Ph_3GeOTeF_5$, $Me_2Ge(OTeF_5)_2$ as well as $Ph_2Ge(OTeF_5)_2$ accessible. Moreover, the Lewis acidity of pentafluoroorthotellurate-based silanes and germanes $R_xE(OTeF_5)_{4-x}$ (x = 3–0, R = aryl, alkyl, E = Si, Ge) was investigated.

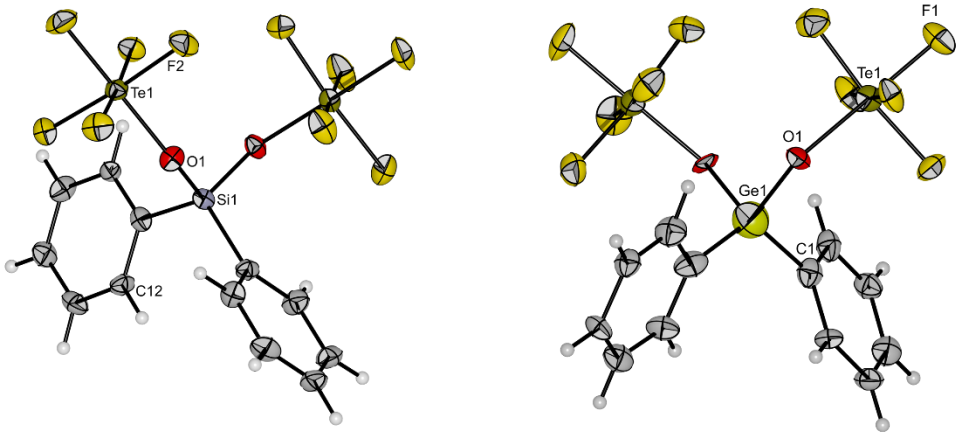

Figure 1: Molecular structure of $Ph_2Si(OTeF_5)_2$ and $Ph_2Ge(OTeF_5)_2$ in the solid state. Thermal ellipsoids are set at 50% probability.

References:

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Anomeric Amide-Enabled Alkene-Arene and Alkene-Alkene Aminative Coupling

Colin Stein[1], Jasper L. Tyler[1], Julius Wiener[1], Florian Boser[1], Constantin G. Daniliuc[1]

Prof. Dr. Frank Glorius[1]

[1] *University of Muenster, Institute of Organic Chemistry, Muenster, Germany*

The development of new C–N coupling reaction has been a focus of extensive research in the past decades. [1] Despite constituting a valuable retrosynthetic transformation, methods to directly form two C–N bonds at a nitrogen center - without relying on heavily prefunctionalized building blocks - remain underdeveloped.[2,3]

In this work we showcase a new method for the aminative coupling of olefins and arenes, or two distinct olefins, directly at nitrogen. We designed a novel anomeric amide reagent, that is able to perform catalyst-free and highly regioselective olefin chloroamination reactions under very mild conditions, thereby inserting a nitrenoid precursor into the target molecule. Subsequent deprotection liberates the active nitrenoid species, which can then undergo intermolecular reactions with a wide variety of nucleophiles, all in a one-pot process.

Due to the simplicity of both the method and its building blocks, high-thoughput experimentation (HTE) was employed to rapidly explore the chemical space. The broad applicability was demonstrated through the modification of pharmaceutically relevant and structurally complex compounds giving rise to high value aziridines and 1,2-chloroamines.

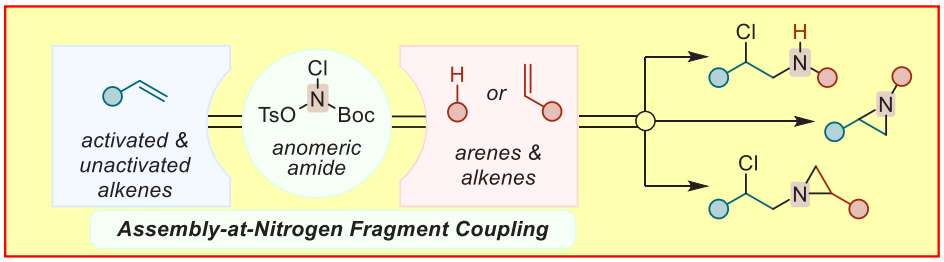

Figure 1: Schematic depiction of the developed anomeric amide-enabled alkene-arene and alkene-alkene aminative coupling.

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[3] P. Onnuch, K. Ramagonolla, R. Y. Liu, *Science* **2024**, *383*, 1019.

DESCOWERY - Deep Eutectic Solvents-enabled Closed and Open-loop Wastes battEry RecYcling -

Matteo Bonomo,[1,2]

[1] *Department of Basic and Applied Science for Engineering, La Sapienza University of Rome, Via del Castro Laurenziano 7, 00161, Rome, Italy*

[2] *National Interuniversity Consortium of Materials Science and Technology (INSTM), Florence, Italy*

Current patterns of energy consumption are closely linked to global warming and climate change. The push toward climate neutrality by 2050 and the transition to a sustainable society depend heavily on harnessing renewable energy, which highlights the pivotal role of batteries in the EU's Green Revolution. In particular, lithium-ion batteries have driven the electronics boom, and their manufacturing is expanding rapidly due to growing demand from electric mobility and large-scale renewable storage. Yet the EU lacks a dependable domestic battery supply chain, with raw materials and production facilities largely located abroad, underscoring the strategic need for recycling to build an alternative, more autonomous supply network. Existing recycling methods (pyro- and hydrometallurgy) fall short on sustainability because they require very high temperatures (PM) or toxic solvents (HM) and involve energy-intensive steps to recover battery-grade materials.

DESCOWERY seeks to create a sustainable recycling route based on Deep Eutectic Solvents (DES), rethinking the entire supply chain. The project aims for a single-stage, energy-efficient regeneration of battery components within a true battery-to-battery closed loop, using tailored DES to selectively extract Li^+ from spent anodes and then employing the Li^+-rich DES to reinsert metals into cathodes. Where battery-grade materials cannot be recovered, DESCOWERY offers a DES-assisted open-loop pathway to produce functional nanoparticles for advanced applications (*e.g.*, sensors, biocides, catalysts).

This innovative approach promises an almost zero-waste, energy-saving recovery process for battery waste, helping to establish a resilient EU supply chain and positioning the Union at the vanguard of the green transition.

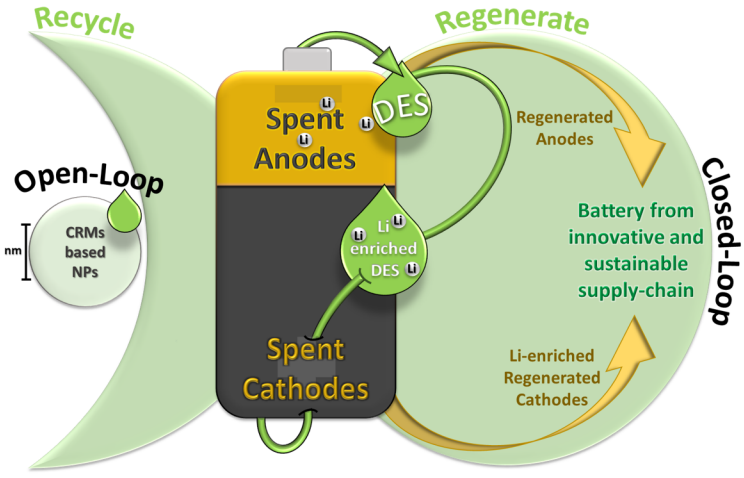

Figure 1: DESCOWERY's concept

Synthesis and Sono-Photochemical Performance of a Non-peripherally Chlorothiophenol-Substituted Zinc Phthalocyanine

Ali Erdoğmuş,[1] Sena Alegöz,[1] Ceren Can Karanlık[1]

[1] *Yildiz Technical University, Department of Chemistry, Davutpaşa Campus, 34220, Esenler, Istanbul, Turkey*

Photodynamic therapy (PDT), sonodynamic therapy (SDT), and their combined modality, sono-photodynamic therapy (SPDT), represent promising minimally invasive strategies for cancer treatment. While PDT relies on light-activated photosensitizers to generate reactive oxygen species (ROS), primarily singlet oxygen ($^1O_2$), SDT utilizes ultrasound irradiation, allowing deeper tissue penetration. Recent studies indicate that SPDT offers synergistic enhancement of ROS production through the simultaneous application of light and ultrasound, leading to improved therapeutic outcomes.[1-3]

Zinc phthalocyanines (ZnPcs) are well-established second-generation photosensitizers due to their strong absorption in the therapeutic window, high photostability, and efficient singlet oxygen generation. In this study, a novel peripherally tetra-substituted zinc phthalocyanine bearing chlorothiophenol groups was synthesized via a single-template cyclotetramerization of 3-nitrophthalonitrile using Zn(II) as the central metal ion. The compound was characterized by FT-IR, mass spectrometry, and UV–Vis spectroscopy.[4,5]

The photochemical, sonochemical, and sono-photochemical singlet oxygen generation efficiencies were systematically evaluated. The results revealed that combined sono-photochemical activation produced significantly higher singlet oxygen levels compared to photochemical activation alone. This enhancement is attributed to ultrasound-induced acoustic cavitation, which promotes intersystem crossing and ROS formation alongside direct photoexcitation. Overall, the synthesized zinc phthalocyanine demonstrates strong potential as an efficient sensitizer for future SPDT-based in vitro and in vivo cancer therapies.

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Coupling voltametric experiments and kinetic Monte Carlo simulations – Insights into hybrid all-Fe redox flow batteries

Alena Neudert,[1,2] Steffen Zappe,[2] Fridolin Röder,[2] Christina Roth[1,2]

[1] *University of Bayreuth, Electrochemical Process Engineering, Bayreuth, Germany*
[2] *University of Bayreuth, Bavarian Center for Battery Technology (BayBatt), Bayreuth, Germany*

The growing demand for renewable energy resources requires durable and inexpensive technologies for large-scale energy storage to balance the fluctuations in power supply.[1,2] In this context, redox flow batteries (RFB) are a promising solution for stationary energy storage due to their scalability, modularity, and long cycle life.[1-3] Compared to the vanadium RFB as the most common technology in the field, the hybrid all-iron RFB offers a more cost-effective, non-toxic and earth-abundant alternative. However, the reduction from iron (II) to iron (0) in the charging process leads to inhomogeneous plating on the electrode and simultaneous parasitic hydrogen evolution reaction (HER).[1] Therefore, the all-Fe RFB requires further improvement and understanding of the ongoing processes.

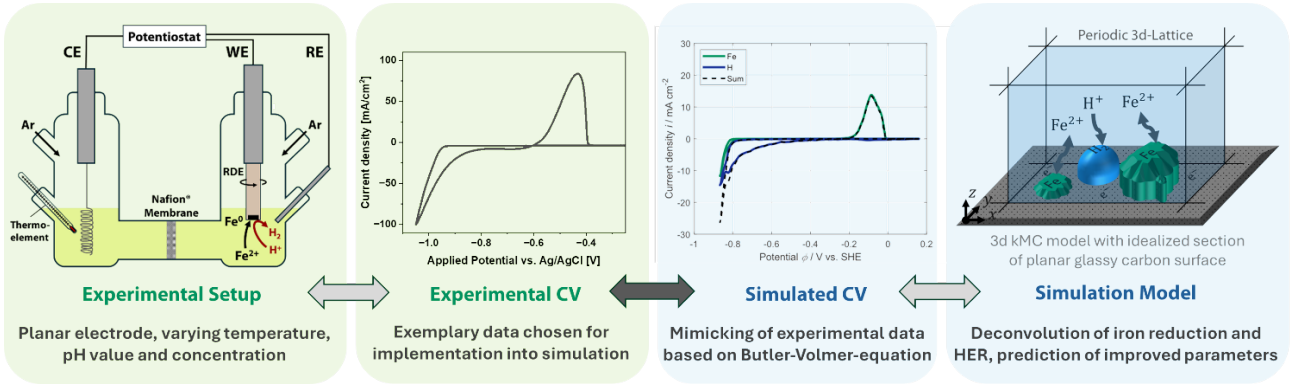

Figure 1: Coupling experiment and simulation by matching cyclic voltammograms (CVs).

We investigated how changes of temperature, iron concentration and pH value affect iron plating and the HER by combining experiments and simulations. The two reduction processes are not separable electrochemically but can be deconvoluted by implementing the experimental data into our kinetic Monte Carlo (kMC) model: After parametrization of the kMC model, the experimental cyclic voltammograms (CVs) are mimicked by a fitted simulation and the model gives insights on and also predicts how hydrogen evolution and the deposition of iron are affected by various combinations of parameters. The approach to couple experiment and simulation enables us to gain fundamental mechanistic insights on the processes taking place on the electrode surface. Suggestions for further improvements to the battery's efficiency include a raise in temperature and a rough surface of the electrode.

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Development of a drone-based measurement system for real-time monitoring of volcanic gas composition at Etna volcano

Antonia Rabe,[1] Niklas Karbach,[1] Nicole Bobrowski,[2,3] Thorsten Hoffmann[1]

[1] *Department of Chemistry, Johannes Gutenberg-University, Mainz, Deutschland*
[2] *University Heidelberg, Heidelberg, Deutschland*
[3] *Instituto Nazionale di Geofisica e Vulcanologia (INGV), Osservatorio Etneo, Catania, Italy*

Volcanic gas emissions provide important insights into magmatic processes beneath the Earth's surface and play a crucial role in assessing volcanic hazards. Depending on their solubility in magma and the respective pressure conditions, volcanic gases are exsolved and released at different depths of a volcanic vent.[1] To study behavior prior to an eruption in hazardous locations, unmanned aerial vehicles (UAVs) offer a safer measurement platform. To increase monitoring frequency, reduce manual labor and the associated risk for the researcher, this work aims to develop a drone station capable of autonomous measurement flights near the volcanic crater.

The sensor system consisting of a SO_2 and CO_2 sensor was developed in-house and can be attached to the drone.[2] To ensure reliable and robust measurement results, a dedicated calibration station was designed and built that allows for easy, repeatable, and automated calibration of the sensor system. The system comprises a pressurized gas container with a calibration gas mixture that connects to a capillary acting as a flow limiter as well as dilution air controlled by a mass flow controller (Fig. 1) that can be adjusted to a defined concentration for sensor calibration at ambient conditions (*p, T, RH*).

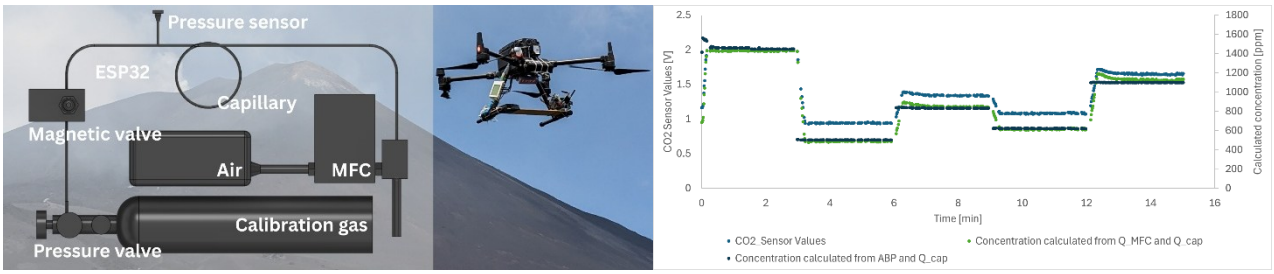

Figure 1: Schematic representation of the calibration station setup (left) and deployed UAV with SO_2/CO_2 gas sensors at Mount Etna (center). The graph (right) shows the calculated, stable calibration concentrations and the corresponding CO_2 sensor response during a five-step calibration.

In order to capture the dynamic behavior of volcanic gas plumes, the UAV-based point measurements are supplemented by a lightweight spectrometer based on a mobile DOAS system.[3] This combination is intended to enable spatially resolved measurements of gas concentrations and fluxes in rapidly changing plume geometries. In the long term, the installation of an autonomous drone docking and charging station at Mount Etna is planned, allowing repeated automated measurement flights and near real-time data acquisition.

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Shape Memory Poly(carbonate urethanes) with high Switching Temperatures for 4D Printing Applications

Theodor Galambos,[1,2] Kerim Temme,[1,2] Thorsten Pretsch,[1]

[1] *Fraunhofer Institute for Applied Polymer Research IAP, Potsdam, Germany*
[2] *University of Potsdam, Institute of Chemistry, Potsdam, Germany*

Shape memory polymers (SMPs) are smart materials capable of recovering a permanent shape upon exposure to an external stimulus such as heat,[1] light,[2] alternating magnetic fields[3] or moisture.[4] However, their use in high-performance sectors like aerospace and automotive is often limited by low switching temperatures, typically below 80 °C. This work focuses on the development of novel thermoplastic poly(carbonate urethanes) (PCUs) with significantly higher and tunable switching temperatures. A key innovation of this work is the demonstration of their suitability for 4D printing via fused filament fabrication (FFF), enabling the direct manufacturing of thermoresponsive objects without requiring a separate programming step.[5] Three PCUs were synthesized with hard segment contents (HSC) of 60, 70, and 80 wt% by reacting a poly(hexamethylene) carbonate diol with 4,4'-methylene diphenyl diisocyanate (MDI) and using the rigid diol isosorbide as a chain extender. The materials were characterized for their thermal, thermomechanical, and mechanical properties. Shape memory performance, including strain fixity and recovery ratios, was assessed in cyclic thermomechanical measurements. The PCUs with HSCs of 60 wt% and 70 wt% were extruded into filaments and used to additively manufacture test specimens to evaluate their 4D printing potential. The glass transition temperature (T_g), which governs the shape memory switching temperature, was successfully tuned by adjusting the HSC, increasing from 72 °C for the lowest HSC up to 136 °C for the highest HSC. All polymers exhibited good thermal stability up to 260°C. All PCUs showed outstanding shape memory properties, with strain fixity ratios (R_f) near 100 % and high strain recovery ratios (R_r) exceeding 86%. Crucially, PCUs with 60 % and 70 % HSC were successfully 4D printed, demonstrating *in-situ* programming where internal stresses from the printing process are stored and later released by heat. The degree of thermoresponsive shrinkage was directly controlled by the printing nozzle. Shrinkage values as high as 63.7 % could be achieved – among the highest reported for 4D-printed thermoplastics.

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Performance investigation of flexible electrodes fabricated using MXene-containing conductive inks for supercapacitor applications

Fatma Altin[1], Ozge Gorduk[1], Semih Gorduk[1], Yucel Sahin[1]

[1]*Yildiz Technical University, Faculty of Arts and Science, Department of Chemistry, Istanbul, Türkiye.*

Energy storage systems have become a major global concern due to increasing industrial and technological demands. The low charging rates and limited lifetimes of commonly used lithium-ion batteries highlight the need for alternative energy storage technologies, such as supercapacitors, that can overcome these limitations [1]. In particular, there is a growing demand for supercapacitors and other flexible energy storage devices that can be integrated with wearable electronics [2]. Flexible electrodes are typically fabricated using conductive inks composed of a solvent, a binder, and a conductive filler. Among these components, the conductive filler plays a critical role, as it significantly influences and enhances electrode performance [3]. Commonly used conductive filler materials include carbon-based materials, metal oxides, metal nanoparticles, and conductive polymers [4]. In this context, the MXene family of two-dimensional materials has attracted considerable attention due to their outstanding electrochemical and mechanical properties. Owing to their unique two-dimensional structure, high electrical conductivity, and tunable surface chemistry, MXenes exhibit great potential for supercapacitor applications. Furthermore, MXenes are rich in surface functional groups, which are considered the primary active sites for energy storage both within the interlayer spaces and at the material surface/interface [5].

In this study, MXene-containing conductive inks will be prepared under optimized conditions and subsequently integrated onto flexible substrates to fabricate flexible electrode materials. The structural, morphological, and compositional characterization of the prepared electrodes will be carried out using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS). The electrochemical performance of the flexible electrodes in supercapacitor systems will be evaluated using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge–discharge (GCD) techniques.

Acknowledgement: This study was derived from a part of the MSc thesis conducted by Fatma Altin in the Department of Chemistry, Faculty of Arts and Science, Yildiz Technical University.

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Connecting Young Chemists: The Role of *Società Chimica Italiana - Gruppo Giovani*

Alice Cappitti, [1] Matteo Bonomo [2]

[1] *Department of Chemistry "Ugo Schiff", University of Florence, 50019 Sesto Fiorentino, Italy*

[2] *Department of Basic and Applied Science for Engineering, La Sapienza University of Rome, Via del Castro Laurenziano 7, 00161, Rome, Italy*

The SCI Giovani (Young Division of the Società Chimica Italiana, SCI) brings together under-35 chemists, including PhD students, postdoctoral researchers, research fellows, professors and young professionals active in academia, research institutions, and industry throughout Italy. With over 1,500 members distributed across the 15 scientific divisions, SCI Giovani represents a large and dynamic community covering all branches of chemistry and closely related interdisciplinary fields.

SCI Giovani supports the scientific and professional development of its members by promoting networking, scientific exchange, and interdisciplinary dialogue through the organization of meetings, workshops, training initiatives, and outreach activities, as well as by fostering interaction with industry and research organizations at both national and international levels.

Among its flagship initiatives, SCI Giovani awards the Premio Primo Levi, aimed at recognizing outstanding research contributions by young chemists. The group also organizes the Y-RICh Workshop (Young Research Ideas in Chemistry), a thematic event focused on emerging research topics and skill development, and the annual MYCS (Merck Young Chemists' Symposium) Congress, which represents the main national forum for young chemists in Italy, fostering scientific discussion, networking, and collaboration across different chemical disciplines.

SCI Giovani is also actively engaged in international cooperation through a growing collaboration with the JCF of the German Chemical Society (GDCh), promoting bilateral scientific exchange and strengthening the European young chemists' community.

The SCI Giovani is active on the main social media platforms; interested readers may follow us by scanning the QR code.

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Preparation of flexible electrodes using conductive ink containing metal-organic framework and investigation of their performance for supercapacitor applications

Melike Dogru[1], Ebrar Dokur[1], Ozge Gorduk[1], Yucel Sahin[1]

[1]Yildiz Technical University, Faculty of Arts and Science, Department of Chemistry, Istanbul, Türkiye.

Portable and wearable electronic devices are widely used in various fields such as microrobotics, health monitoring, rehabilitation, and motion sensing.[1] For the efficient operation of these devices, flexible energy storage systems that are compact, lightweight, mechanically robust, and exhibit superior electrochemical performance are required. Owing to their mechanical flexibility, high safety, and durability, flexible supercapacitors have become a significant research focus in recent years.[2] In addition, flexible supercapacitors are an essential technology for sustainable energy systems thanks to their long cycle lives and fast charge-discharge capabilities. Flexible supercapacitors are high-capacity, low-internal-resistance energy storage systems that can store and transmit energy at relatively higher rates compared to batteries, thanks to an energy storage mechanism involving simple charge separation at the interface between the electrode and the electrolyte.

The performance of flexible supercapacitors is affected by factors such as the type of electrode and electrolyte materials used, electrode-electrolyte interface properties, conductivity, and active surface area. To achieve high electrical conductivity, elevated energy density, and long cycle life in flexible supercapacitors, extensive research has been conducted on the formulation of conductive inks.[3] Conductive inks are typically formulated by homogeneously dispersing metal nanoparticles that provide electrical conductivity and catalytic activity, polymers serving as binders, and carbon allotropes acting as conductive fillers within a suitable solvent medium.[4]

Therefore, in this study, conductive inks were formulated using metal–organic framework (MOF) materials with high porosity and superior capacitive properties, and a flexible supercapacitor was designed employing the prepared conductive inks. Morphological and structural characteristics of flexible electrodes were investigated using techniques such as scanning electron microscopy, energy-dispersive X-ray spectroscopy, and Fourier transform infrared spectroscopy. To evaluate the performance of the fabricated flexible electrodes in supercapacitor applications, cyclic voltammetry, electrochemical impedance spectroscopy, and galvanostatic charge-discharge tests were performed.

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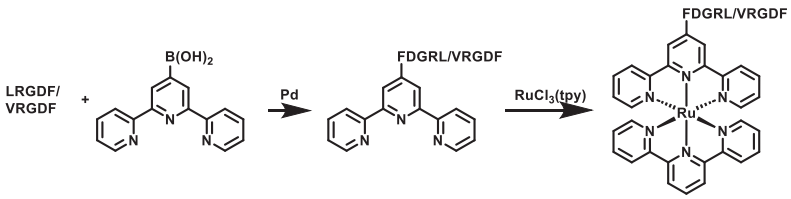
Mechanochemical synthesis of ruthenium bioconjugate complexes

Dominik Gilbert,[1] Steffi Krause Hinojosa,[1] Lars Borchardt,[1]

[1] *Ruhr-University Bochum, Inorganic Chemistry, Bochum, Germany*

With increasing numbers of people ailing with cancer, the field of anti-cancer ruthenium complexes, is raising.[1] Ruthenium polypyridyl complexes exhibit unique properties due to their ability to absorb light in the UV/vis spectrum, and a high lipophilicity is essential to enable membrane penetration and reactivity at the desired intracellular location. A new upcoming way of increasing the lipophilicity is to use peptides and could be used these types of complexes to increase cellular uptake.[2] Synthesis routes for these complexes are time consuming and need high amounts of solvents due to the low solubility of bioconjugates. The relative instability of most bioconjugates towards acids, bases, reduction, oxidation and temperature together with the light sensitivity of ruthenium complexes make them quite difficult to handle. Therefore, an uprising method for the synthesis of ruthenium bioconjugate complexes is the use of mechanochemistry. By using mechanochemistry with a resonant acoustic mixer (RAM) bioconjugates in form of peptides can be synthesized. The relatively low solubility of peptides in any solvents becomes obsolete for the solid-state reactions in a RAM device which as well can reduce the reaction time needed for peptide synthesis to mere minutes. [3] By using the RAM, the reaction conditions are also comparatively mild resulting in a lowered risk of bond breakage of the bioconjugate. Here we focus on the mechanochemical synthesis of the peptides consisting of LRGDF (Leucin-Arginine-Glycine-Aspartic acid-Phenylalanine) and VRGDF (Valine- Arginine-Glycine-Aspartic acid-Phenylalanine). Phenylalanine is iodinated in *para* position to undergo a direct mechano-catalysed Suzuki reaction with terpyridine boronic acid. The RGD sequence is required for receptor recognition. As well as a ruthenium terpyridine precursor which will then be combined by using mechanochemistry to synthesize novel ruthenium bioconjugate complexes. [4] The peptide as well as the precursor ($RuCl_3$(tpy)) were synthesized successfully.



Scheme 1: Reaction scheme of further steps which will be done in the near future.

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Helicene-fused BODIPYs as CPL Emitters

Anselm Uhlmann,[1] Daniel B. Werz[1]

[1] *University of Freiburg, Institute for Organic Chemistry, Freiburg, Germany*

Fluorescent dyes have demonstrated considerable utility in a multitude of fields. Their applications encompass optical devices such as lasers[1] and LEDs[2], energy production (e.g., in solar cells)[3], and a vast array of analytical techniques, including bioimaging[4] and chemical sensing[5]. Additionally, they play a pivotal role in numerous pharmaceutical applications, particularly in diagnostics[6] and photodynamic therapy[7]. The introduction of chirality into these dyes provides a novel means of utilizing their distinctive and tunable chiroptical properties. These molecules can be employed in screens[8], stereo dependent analytic techniques or circular polarized lasers[9].

The objective of this project is to synthesize end-on helicene-fused BODIPYs. Upon successful synthesis and separation of the enantiomers, the investigation of their chiroptical properties and thus their potential applications in optical devices are the main focus of this work. The general synthetic strategy to obtain such helicene-fused BODIPYs is shown in figure 1. Once this objective is achieved, the incorporation of helicenes of varying sizes and their influence on the resulting optical properties of these system will be investigated. A specific focus lies on tuning the emission wavelength to achieve near infrared fluorescence.

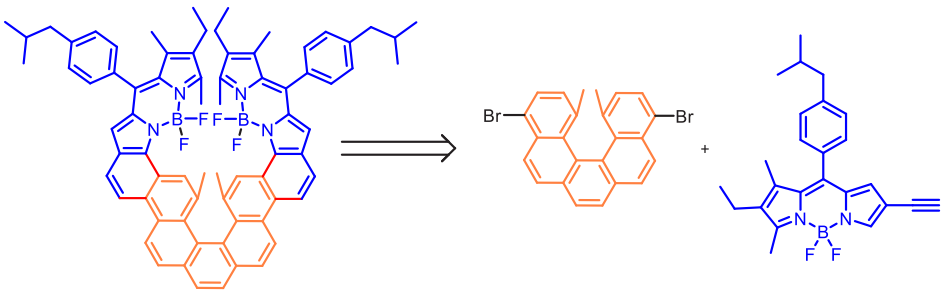

Figure 1: General synthetic strategy to obtain end-on helicene-fused BODIPYs.

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Stereospecific Insertion of Cyclic Amidines into Aryl-Substituted Cyclopropanones: Access to Complex Spirocyclic Aminals

Richard Herzog,[1] Ishika Agrawal,[1] Heinrich F. von Köller,[1] Konstantin Kloiber,[2] Daniel B. Werz[1]

[1] *University of Freiburg, Institute of Organic Chemistry, Freiburg, Germany*

[2] *University of Freiburg, Institute of Inorganic Chemistry, Freiburg, Germany*

Cyclopropanones are the simplest cyclic ketones and due to their high ring strain and thus reactivity increasingly utilized as three-carbon building blocks in organic synthesis.[1,2] As cyclopropanones are known to readily undergo hydrolysis and oligomerization reactions they are usually stored as bench-stable sulfonylcyclopropanols (SCPs). The latter may then be liberated in situ to the corresponding cyclopropanones upon addition of base.[3] In this work a facile, catalyst-free protocol to accessing structurally complex, spirocyclic aminals from cyclopropanone surrogates and amidines is reported.[4] The two-component reaction is described as a stereospecific insertion of the amidine CN double bond into the C1-C2 bond of the cyclopropanone via *N*-addition to the carbonyl group, followed by ring-enlargement. The products display similarities to numerous biologically active oligocyclic systems. Further structural diversification is demonstrated and a proposed mechanism is provided based on experimental and computational evidence.

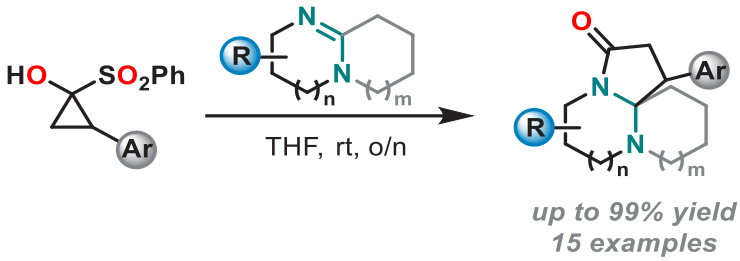

Figure 1: Reaction of in situ generated cyclopropanones with bicyclic amidines to tricyclic, fused *N*-containing spirocyclic aminals.

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Presenting youngSCS: The Swiss Young Chemists' Network

Lukas Schlemper,[1] Marie-Désirée Schlemper-Scheidt,[2] Helena Solé Àvila[3]

[1] *ETH Zürich, Laboratorium für Organische Chemie, Zürich, Switzerland*

[2] *Université de Neuchâtel, Institute of Chemistry, Neuchâtel, Switzerland*

[3] *EPFL, Laboratory of Catalysis and Organic Synthesis, Lausanne, Switzerland*

The youngSCS is the youth division of the Swiss Chemical Society (SCS) and it was founded with three central goals. In the first place, the youngSCS aims to provide a network for young researchers to meet in an informal setting and learn from each other. Secondly, we aim to establish and maintain good contacts with our partner societies in neighbouring countries and internationally, to foster a lively exchange between chemists form different backgrounds and cultures. Lastly, the youngSCS attempts to facilitate access for young researchers to the chemical industry.



Figure 1: Overview of all institutes that are represented in the youngSCS.

To achieve these goals, the youngSCS is involved in multiple events and collaborations. For example, the annual Swiss Snow Symposium, a three-day conference, where a wide range of chemical research fields are represented, including speakers from various companies. Moreover, the youngSCS is represented in the EYCN and the IYCN via its delegates. We organize a wide range of company visits each year to forge contacts between young researchers and industry representatives. Visits between different institutes to connect people across the country are also happening on a regular basis.

A successful and ongoing collaboration between us and the SCS is the "Mentoring Program", where young chemists are brought into contact with more experienced and well-established mentors, who are giving advise on how a career might progress and what decisions and career paths entail.

As the EYCN delegates we would like to present the youngSCS at the JCF spring symposium to build and foster lasting contacts and exchanges with the present members of the chemical society.

Alkyne-Tagged Imidazolium-Based Membrane Cholesterol Analogs for Raman Imaging Applications

Sophie Korgitzsch,[1] Constanze Schultz,[2] Tristan Wegner,[1] Corinna Heusel,[1] Tim Gallagher,[1] Yanjun Zheng,[3] Marcus Werner,[4] Seraphine V. Wegner,[3] Tobias Meyer-Zedler,[2,5] Oliver Werz,[4] Michael Schmitt,[5] Juergen Popp[2,5] and Frank Glorius[1]

[1] *University of Münster, Institute of Organic Chemistry, Münster, Germany*
[2] *Leibniz Institute of Photonic Technology (Leibniz-IPHT), Jena, Germany*
[3] *University of Münster, Institute of Physiological Chemistry, Münster, Germany*
[4] *Friedrich-Schiller-University Jena, Institute of Pharmacy, Jena, Germany*
[5] *Friedrich-Schiller-University Jena, Institute of Physical Chemistry (IPC), Jena, Germany*

Cholesterol plays a crucial role in mediating essential cellular processes as well as maintaining the structural integrity of most eukaryotic membranes. Due to its vast biological relevance, strategies to investigate cholesterol-mediated biological processes are of high interest. Current approaches often rely on fluorescently labelled cholesterol analogs which commonly modify the amphiphilic character or add steric bulk in the backbone, obstructing natural membrane integration. Improved tools for cholesterol imaging are thus needed.[1,2]

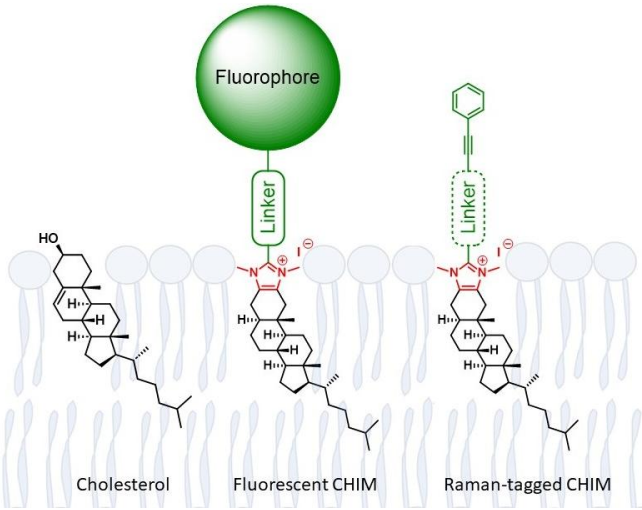

Figure 1: Molecular structure and schematic depiction of the membrane integration of natural cholesterol and fluorescently labelled CHIM as well as the herein investigated Raman-tagged analog.

In our work, we report a series of alkyne-tagged imidazolium-based cholesterol analogs (CHIMs) observable by Raman spectroscopy allowing for cellular multiplexed Raman imaging in HEK cells.[1] For CHIMs, the hydroxy group of natural cholesterol is replaced with an imidazolium moiety, preserving the amphiphilic nature of cholesterol.[2] By functionalizing the imidazolium group in the C2 position, reporter molecules point into the extracellular matrix. In combination with using more compact Raman tags, the disruption of natural membrane integration and cellular interactions is minimized. Therefore, we envision Raman-tagged CHIMs to be a promising tool for the investigation of cholesterol-mediated cellular processes complementary to other established methods.

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Synthesis of amine-functionalized 1,3-bis(2-arylimino)isoindolines and their derivatives

Umay Yıldırım,[1] Burak Yıldız,[2] M. Kasım Şener,[1]

[1] *Yıldız Technical University, Department of Chemistry, 34210 Esenler, İstanbul, Türkiye*
[2] *Ege University, Program of Refinery and Petrochemical Technology, 35800 Aliağa, İzmir, Türkiye*

1,3-bis(2-arylimino)isoindolines (BAI) are robust, tridentate ligands that coordinate to metal centers through a rigid N,N,N-donor set. Their planar molecular architecture provides exceptional thermal stability and tunable electronic properties. This study presents the synthesis of novel amine-functionalized BAI derivatives via systematic R-group modifications (Fig. 1). This structural functionalization significantly alters the solubility and donor capabilities of the ligands. The strategic incorporation of amine functionalities not only modulates the electronic density of the central isoindoline core but also provides a versatile handle for further chemical derivatization and the development of hybrid materials. The resulting metal complexes exhibit adjustable photophysical characteristics promising for optical materials. Furthermore, the functionalized structure suggests utility in electrochemical systems and biomimetic catalysis. By establishing a fundamental understanding of these structure-property relationships, this research paves the way for the design of next-generation multifunctional materials.[1-4]

Acknowledgement: This study was derived from a part of MSc thesis conducted by Umay Yıldırım in the Department of Chemistry, Faculty of Arts and Sciences, Yıldız Technical University.

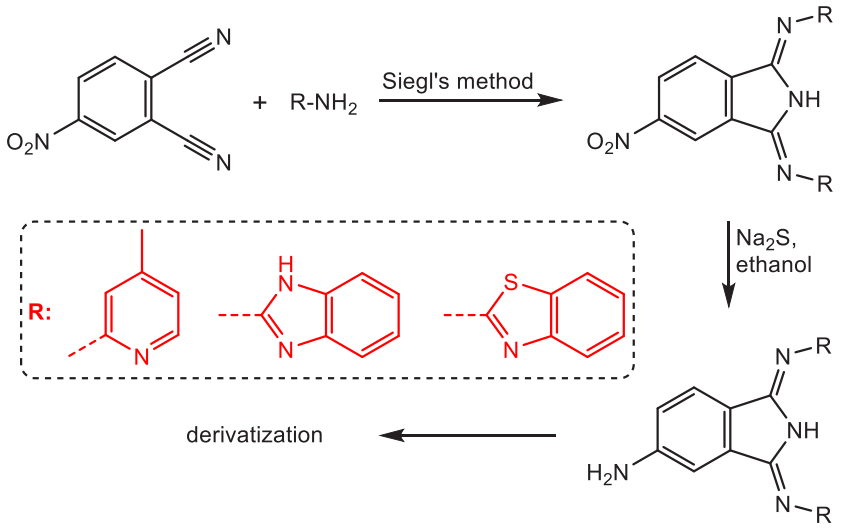

Figure 1: Synthesis of amine-functionalized 1,3-bis(2-arylimino)isoindolines.

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Catalytic Upcycling of Polyolefins Waste using Ru/Al_2O_3 catalyst

Antonio Cosimo Pio Trimboli,[1] Emilia Paone,[1] Riccardo Pellegrini,[2] Elena Clara Groppo,[3] Sven Gratz,[4] Francesco Mauriello,[1] Lars Borchardt[4]

[1]Dipartimento di Ingegneria Civile, Energia, Ambiente e Materiali (DICEAM), Università degli Studi Mediterranea di Reggio Calabria, Via Zehender (già via Graziella) - Loc. Feo di Vito, I-89123 Reggio di Calabria (RC) Italy

[2]Chimet S.p.A., Via di Pescaiola n. 74, I-52041 Viciomaggio (AR) Italy

[3]Department of Chemistry, NIS Centre and INSTM, Università degli Studi di Torino, Via Quarello n. 15, I-10135 Torino, Italy

[4] Inorganic Chemistry I, Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany

Global plastic production exceeds 400 million tons per year, with polyolefins (POs) dominating both virgin plastics and post-consumer waste. In Europe, despite strong circular-economy policies, over 95% of post-consumer POs are still discarded, highlighting the limitations of current recycling strategies.[1] Mechanical recycling often leads to material downgrading, while chemical routes typically rely on energy-intensive thermal cracking or high-pressure hydrogenation. Here, we develop catalytic and mechanochemical approaches for the reductive upcycling of polyolefins into value-added liquid hydrocarbons under mild, hydrogen-free conditions. Polyethylene (PE) is efficiently converted using a commercial Ru/Al_2O_3 catalyst under inert atmosphere in the presence of hydrogen-donor alcohols. Among those tested, 2-propanol affords the highest PE conversion (up to 65%) and high selectivity toward C_{12}–C_{20} liquid hydrocarbons with minimal gas formation (<5%). The alcohol acts both as reaction medium, improving polymer diffusion and mass transfer, and as an in situ hydrogen donor, eliminating the need for external H_2. Negligible conversion in the absence of 2-propanol underscores the critical role of the liquid phase.[2] To further improve sustainability, thermal input is replaced by mechanical energy.[3] We present the first systematic comparison of several mechanochemical platforms for PE upcycling using Ru/Al_2O_3 and 2-propanol. The impact-driven mixer mill shows the best performance, reaching 30% conversion after 6 h and 96% selectivity toward C_5–C_{20} liquid hydrocarbons without external heating or pressure. The methodology is successfully extended to real post-consumer polyolefin waste. Overall, this work reveals a strong interplay between catalyst design, hydrogen-transfer chemistry, and mechanical activation, offering an energy-efficient and scalable route for polyolefin upcycling aligned with circular plastics strategies.

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P140

Designing Polymeric Adsorbents for Sustainable PFAS Remediation

Ahmet Cetinkaya,[1] Belkacem Tarek Benkhaled,[1] Mona Semsarilar[1]

[1] *Institut Européen des Membranes—IEM UMR 5635, Univ Montpellier, CNRS, ENSCM, 34090 Montpellier*

Per- and polyfluoroalkyl substances (PFAS) are highly persistent environmental contaminants due to the exceptional thermal and chemical stability of the carbon–fluorine bond. [1,2] Their widespread occurrence in water sources poses significant risks to human health, including hepatotoxicity, endocrine disruption, and immune system impairment, as well as serious ecological impacts. [3] The hydrophobic and lipophilic nature of PFAS makes them difficult to remove using conventional water treatment technologies, highlighting the urgent need for selective, sustainable, and reusable remediation strategies. [4]

In this work, we report the development of polymeric adsorbent materials with potential for selectively removing PFAS with diverse functional groups and chain lengths, which are also reusable and potentially scalable for industrial applications. Representative systems include crosslinked hybrid-hydrogels which can be tailored to target different PFAS compounds. These materials are straightforward and cost-effective to produce, offering high adsorption efficiency and reusability, providing a solid foundation for the development of sustainable and practical water treatment solutions capable of mitigating PFAS contamination and ensuring access to safe water.

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P141

26th Frankfurt Career Fair for STEM

Badria Ali, Annabelle Brauel, Leon Kirschner, Lena Kemper, Nils Wegerich

JCF Regional Network Frankfurt am Main

Save the date for November 4th and 5th, 2026! The 26th annual Frankfurt Career Fair for STEM (Frankfurter Jobbörse für Naturwissenschaftler:innen) will take place again. The program begins on Wednesday, November 5, with plenty of workshops and seminars. You will also have the opportunity to have your application documents and CVs reviewed by trained career consultants. You can find out more about the various events at jobboerse-ffm.de. Registration is expected to begin in early October.

On Thursday, November 5, the career fair will take place, with more than 20 companies and associations participating. From 9:30 a.m. to 4:30 p.m., companies from the chemical, pharmaceutical, and life science industries, as well as start-ups, business consultancies, and patent law firms will exhibit. In addition to classic exhibition stands, many companies will give short presentations about their businesses. There will also be an opportunity to have professional application photos taken. The program will conclude with a public job interview that you can attend live.





The Chemiker Spaß Gesellschaft (CSG) Bayreuth

Moritz Riegler[1]

[1] *University of Bayreuth, Bayreuth, Germany*

The Chemiker Spaß Gesellschaft (CSG), the official alumni association of chemistry at the University of Bayreuth, together with the JCF Bayreuth, shapes the scientific and social life of the chemical community at the University of Bayreuth. Founded in 2008, the CSG has more than 500 members and serves as a bridge between alumni and students. Through lectures, mentoring programs, and social activities, it fosters exchange among students, doctoral candidates, alumni, and professors. A flagship event is the Chemistry Graduation Day, during which bachelor's, master's, and doctoral graduates are honored in a festive ceremony and recognized with awards from the Otto Warburg Foundation. In addition, the CSG collaborates with schools by awarding prizes for outstanding seminar papers and promoting the study of chemistry.

Furthermore, the association organizes the annual "Himmelfahrtskommando" (a hiking event on Ascension Day), a dodgeball tournament with more than 100 chemists, and a rubber boot throwing competition. The CSG also offers professional development activities such as the FT Seminar, in which key large-scale instruments available in the chemistry department at the University of Bayreuth are presented in an accessible manner to inform participants about new research opportunities. Through fundraising and donation campaigns, the CSG regularly supports charitable organizations, thereby linking social engagement with student life.

Another major focus is public outreach. At events such as Campus Erleben, Girls' Day, and school outreach days, the CSG represents chemistry through hands-on experiments, demonstration lectures, and interactive activities. Overall, the CSG e.V. makes a significant contribution to networking, early-career support, and the visibility of chemistry in Bayreuth.

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Optical Signatures of CuIn-Based Quantum Dots in Bio-Inspired Hybrid Systems

Özge İbiş, [1], Caner Ünlü, [1]*

[1] *Istanbul Technical University, Department of Chemistry, İstanbul, Türkiye*

Photosynthesis is one of the most fundamental processes sustaining life on Earth, enabling plants, algae, and cyanobacteria to convert solar energy into chemical energy through the fixation of CO_2 and water, producing carbohydrates and molecular oxygen. Despite its central role in global energy and carbon cycles, natural photosynthesis utilizes only a limited fraction of the solar spectrum and is highly sensitive to environmental stress factors.

Quantum dots are semiconductor nanocrystals typically ranging from 1.5 to 10 nm in size, whose optical and electronic properties are governed by quantum confinement effects. As zero-dimensional materials, their band gap energies and emission characteristics can be precisely tuned by controlling size, shape, and composition, leading to size-dependent color emission. These unique and customizable properties have established quantum dots as an important class of functional nanomaterials in light-harvesting and optoelectronic applications.

In natural photosynthesis, light absorption is largely confined to the visible region, while fluctuations in light intensity, UV radiation, and environmental stress can impair photosynthetic performance and damage pigment–protein complexes. In this context, quantum dots and related nanomaterials have attracted growing interest as optical modifiers, capable of extending spectral utilization and mitigating harmful radiation effects, thereby offering new strategies for enhancing or complementing photosynthetic light harvesting. [1, 2]

In this concept heavy metal free - colloidal quantum dots (QDs) of IIB–VIA which have been synthesized through environmentally friendly methods and interactions of these QDs with photosynthetic systems were investigated through in vitro studies to better understand their effects on plants.

Ultimately, this work seeks to explore strategies for modulating photosynthesis by enhancing light-harvesting efficiency, increasing photosynthetic product formation, and protecting photosynthetic pigments from the adverse effects of ultraviolet radiation.

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Photoswitchable Ligands Enable Thermodynamic Disequilibration of Metal-Organic Assemblies

Maximilian J. Notheis,[1] Dr. Larissa K. S. von Krbek[1]

[1]*University of Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Bonn, Germany*

A fundamental understanding of how to access and sustain meta-stable states in artificial systems and materials is a step towards extending life-like behaviours to inanimate objects, opening numerous perspectives from more sustainable self-repairing materials to medical applications in targeted drug release.

A one-pot sub-component self-assembly using a photoresponsive building block resulted in selective formation of high-fidelity heterobimetallic helicates. Investigating the photoresponsive behavior of the helicates revealed a light-driven energy-ratchet mechanism. Continuous white-light irradiation operates the energy ratchet autonomously by exciting both switching transitions simultaneously. This amplifies a minor photostationary state into a dominant, long-lived meta-stable diastereomer. Additionally, operation of the ratchet accelerates regioselective metal-cation exchange (Zn_2**L** → ZnFe**L**), providing spatiotemporal control over selective metal ion capture.

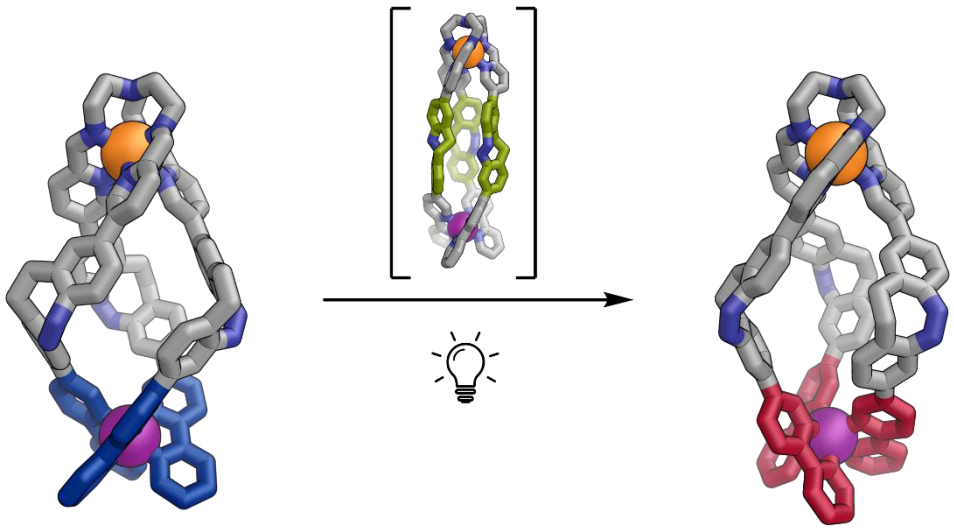

Figure 1: Exposure to white light selectively inverts the stereochemistry of an octahedral metal site through an energy ratchet mechanism, accumulating a meta-stable diastereomer.

This work shows that light driven reaction networks, specifically energy ratchets, are a foundational tool to accumulate meta stable states in self-assembled metal-organic structures and that the innate energy of these states can be harnessed for function.[1]

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Assessing the Future Orientation of School Chemistry

Edwin Bogdan,[1] Thomas Waitz[2]

[1] *Georg-August-Universität, Institute of Inorganic Chemistry, Department of Chemistry Education, Göttingen, Germany*

In the context of diverse challenges facing humanity today, sciences are concerned with proposing solutions to overcome them. Chemistry contributes substantially through the continuous advancement of materials, processes, and technologies. Despite the potential of technologies to enhance the future-oriented nature of chemistry education, their systematic integration into chemical school curricula remains doubtful, particularly within the German education system. This is noteworthy, as education should connect learning contents with technological developments that are likely to influence students' future professional and everyday environment.[1]

The present contribution first outlines key characteristics of emerging technologies[2] and discusses their current consideration within chemical curricula and teacher education. Building on this analysis, experimental approaches for chemistry class and student laboratories are presented. These experiments are linked to emerging technologies identified by IUPAC[3] and are intended to demonstrate how cutting-edge innovations can be integrated into science education to foster a deeper understanding of modern chemistry.

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[6]Cyclo-*para*-azulenylene

Clara Douglas,[1] Oliver Dumele[1]

[1] *University of Cologne, Department of Chemistry, Cologne, Germany*

Nonalternant hydrocarbons differ significantly from their alternant analogs due to their asymmetric electronic structure, which manifest in distinct (anti)aromaticity, optical behavior, and redox properties.[1,2] Subjecting such systems to strain further changes these characteristics. Azulene, a nonalternant hydrocarbon known for its anti-Kasha fluorescence and intense blue colororation, is herein strained into a macrocycle along its 2,6 positions, forming the symmetric azulene analogue of [6]cycloparaphenylene, termed [6]cycloparazulenylene (**[6]CPA**). Its structure was elucidated via single-crystal X-ray diffraction, revealing pronounced dihedral torsion between adjacent azulene units and an unusual corkscrew-like tubular packing motif. The macrocycle demonstrates electronic delocalization along the macrocyclic perimeter, a remarkably narrow HOMO–LUMO gap, and intense absorption in the visible range. Computational analyses of aromaticity show that, despite the 60 π-electron (4n) macrocyclic perimeter, the overall electronic structure is dominated by the local aromaticity of the 10 π-electron (4n+2) azulene subunits, while a weak paratropic ring current is induced upon application of an external magnetic field. **[6]CPA** represents the first all-azulene carbon nanohoop and the first cyclic architecture constructed solely from azulene units.

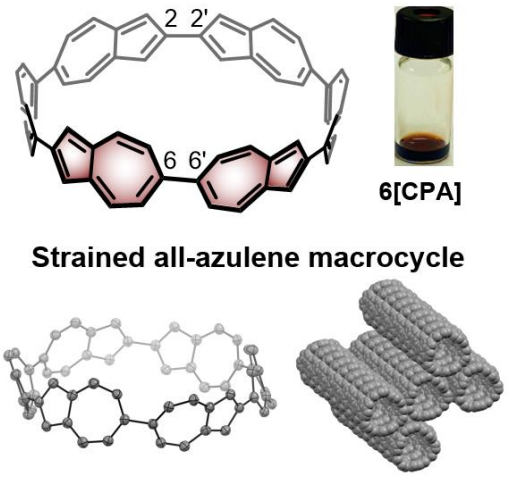

Figure 1: Molecular structure, single-crystal X-ray structure and packing of **[6]CPA**.

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Purely equatorial lasing in spherical liquid crystal polymer microlasers with engineered refractive index gradient

David Ripp,[1] Nachiket Pathak,[1] Vera M. Titze,[1,2] Andreas Mischok,[1] Marcel Schubert[1]

[1] *University of Cologne, Humboldt Centre for Nano and Biophotonics, Department of Chemistry and Biochemistry, Cologne, Germany.*

[2] *Max Planck Institute of Colloids and Interfaces, Department of Sustainable and Bio-inspired Materials, Potsdam, Germany*

Whispering gallery mode (WGM) microlasers show high sensitivity to external stimuli and distinct spectral features, making them particularly attractive for various sensing applications as well as for cell tagging and tracking, respectively.[1–3] Liquid crystal WGM microlasers further provide intrinsic anisotropic optical properties that can be used to shape and manipulate light even inside spatially highly symmetric structures.

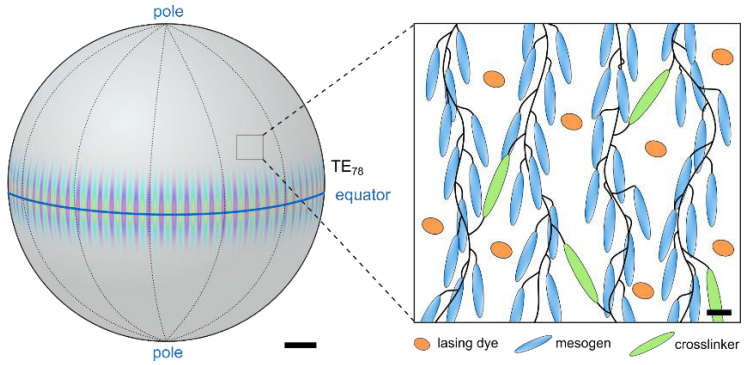

Figure 1: Illustration of a microlaser and the TE78 WGM (trapped light that travels at the inner surface of the sphere) confined to the equatorial plane. Scale bar, 1 µm. The zoomed-in area shows an illustration of the molecular structure of the liquid crystal polymer. Scale bar, ~1 nm.

Here, we present the fabrication and detailed optical characterization of a spherical bipolar liquid crystal polymer microlaser that tightly confines the optical path of WGMs to the equatorial plane.[4] Controlled anchoring of the liquid crystal mesogens followed by polymerization forms a fixed refractive index (RI) gradient within the spherical microcavity. We further show that the RI gradient induces a characteristic spectral splitting of the lasing modes. By combining hyperspectral imaging and analytical modeling, we attribute this effect to the lifting of the energy degeneracy of azimuthal laser modes, providing direct insights into the complex interplay between RI gradients and WGM confinement. Single plane confinement of lasing within a spherical microbead enables robust and spatially localized sensing, particularly advantageous for fast point scanning microscopy or in highly dynamic biological environments.

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Electrochemiluminescence based on the formation of exciplex/excimer

Chang-Ki Moon[1,2], Yuka Yasuda[3], Yu Kusakabe[3], Anna Popczyk[1], Shohei Fukushima[3], Julian F. Butscher[1], Nachiket Pathak[1], Joel Schlecht[4], Kuraudo Ishihara[3], Oliver Dumele4, Hironori Kaji[3], Malte C. Gather

[1] *Humboldt Centre for Nano- and Biophotonics, Department of Chemistry and Biochemistry, University of Cologne, Cologne, Germany*

[2] *Organic Semiconductor Centre, School of Physics and Astronomy, University of St Andrews, St Andrews, United Kingdom*

[3] *Institute for Chemical Research, Kyoto University, Uji, Kyoto, Japan*

[4] *Institute of Organic Chemistry, Department of Chemistry and Biochemistry, University of Cologne, Cologne, Germany*

Used extensively in sensing applications, the application of solution-state electrochemiluminescent (ECL) devices, often referred to “fluid light”, in lighting and displays has been constrained by their low luminance and short operational lifetime. Here, we introduce ECL mechanisms based on exciplex[1] and excimer formations[2], leading to a significant improvement in the luminance, efficiency, and operational longevity of ECL devices, and demonstrate its use in a calligraphic display (Figure 1a). Electrochemically induced hyperfluorescence (ECiHF) is achieved by using “double-decker” arrangement assumed by the electron donor and acceptor segments of the molecule TpAT-tFFO to realize thermally activated delayed fluorescence from an electrogenerated charge-transfer excimer state (Figure 1b) and a subsequent energy transfer to the rubrene emitter TBRb.

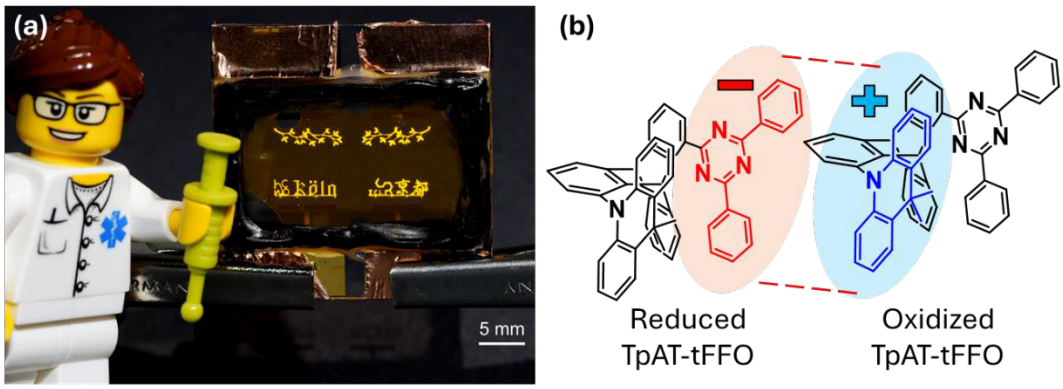

Figure 1. (a) Calligraphic display based on ECL. (b) CT excimer formation between reduced and oxidize TpAT-tFFO.

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Reducing the threshold of organic polariton lasers by lateral confinement

Julia Witt[1], Jiwoo Oh[3], Tommaso Marcato[3], Andreas Mischok[1], Chih-Jen Shih[3*], Malte C. Gather[1,2*]

[1] *Humboldt Centre for Nano- and Biophotonics, Department of Chemistry and Biochemistry, University of Cologne, Greinstr. 4-6, 50939 Cologne, Germany*

[2] *Organic Semiconductor Centre, SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews KY16 9SS, United Kingdom*

[3] *Institute for Chemical and Bioengineering, ETH Zürich, 8093 Zürich, Switzerland*

Organic polariton lasers are promising sources of coherent light. They operate at room temperature and, unlike photon lasers, they do not necessarily require population inversion. For this reason, they can potentially have lower lasing thresholds and therefore may require less driving energy.

The blue fluorescent organic dye 4,4-bis[(N-carbazole)-styryl]biphenyl (BSBCz) shows excellent lasing properties in conventional lasers and is highly promising for electrically pumped laser diodes. Here, we realize polariton lasers by sandwiching BSBCz between two highly-reflective Bragg mirrors and analyze the threshold of these lasers. By doping BSBCz into 4,4′-Bis(N-carbazolyl)-1,1′-biphenyl (CBP), we achieve polariton lasing thresholds down to 8.7 pJ/μm^2.[1] By miniaturizing the active area of the laser and thus introduction lateral polariton confinement, we further lowered the lasing threshold down to 0.2 pJ/μm^2. The isolated organic dots were fabricated by co-evaporation through ultra-thin shadow masks. With this method, dots with a diameter down to 5 μm could be fabricated showing nearly no shadowing effect. These results demonstrate that BSBCz can be optimized for polariton lasing and lasing threshold can be reduced significantly, which is essential to get a step closer to an electrically pumped polariton laser.

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Peptide inhibitors target the TANGO1–cTAGE5 complex to reduce collagen secretion in dermal fibroblasts

Melina Ruppel[1], Anna Bornikoel[2], Beate Eckes[2], Thomas Krieg[2], Vivek Malhotra[3], Ishier Raote[4], Ines Neundorf[1]

[1] University of Cologne, Institute of Biochemistry, Cologne, Germany
[2] University Clinic Cologne, Institute of Biochemistry, Cologne, Germany
[3] Centre for Genomic Regulation, Institute of Science & Technology, Barcelona, Spain
[4] Université Paris Cité, Institute Jacques Monod, Paris, France

The extracellular matrix (ECM) is a dynamic network essential for cellular architecture, signaling, and tissue homeostasis. The primary constituent of both the extracellular matrix and fibrotic scar tissue is fibrillar collagens.[1] Excessive secretion of ECM proteins, most prominently collagen, is a key driver of fibrotic diseases such as Scleroderma, which is characterized by skin thickening, joint immobility, muscle weakness, and progressive loss of organ function.[2] Because effective antifibrotic therapies remain limited, targeting collagen secretion is of high interest.

The Transport and Golgi organization 1 (TANGO1) protein family has emerged as a key organizer of ER exit sites, forming transient inter-organelle tunnels via their ER luminal part. A crucial step in the secretory pathways involves the interaction of the coiled-coil 2 domains of TANGO1 with its paralog cutaneous T-cell lymphoma-associated antigen 5 (cTAGE5). This interaction initiates the formation of coat protein complex II (COPII)-coated vesicles, transferring collagen and ECM components to the extracellular space. Due to the critical role of TANGO1 proteins in collagen trafficking, their functional inhibition offers a promising strategy to reduce collagen hypersecretion.[3]

We develop peptide-based inhibitors that selectively disrupt the interaction between TANGO1 and cTAGE5. To this end, we designed and synthesized peptide inhibitors incorporating a TANGO1 or cTAGE5-derived binding motif fused to the cell penetrating peptide sC18*. These constructs were evaluated for cytotoxicity, cellular uptake, and their effects on collagen I secretion in dermal fibroblasts. Our findings demonstrate that targeted interference with the TANGO1-cTAGE5 complex using cell-penetrating peptide inhibitors effectively reduces collagen I secretion. This approach highlights a promising therapeutic strategy to modulate ECM deposition and possibly reduce the progression of fibrotic disease.

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Xanthone Carboxylic Acids as Modular Scaffolds for Photoactivatable Artemisinin Dyads

Jan F. W. van Stiphoudt,[1] Leon F. Klefisch,[1] Axel G. Griesbeck[1]

[1] *University of Cologne, Institute of Organic Chemistry, Cologne, Germany*

Artemisinin is a natural compound that has been used in medicine for decades. It plays a key role in the treatment of malaria, and extensive research has explored its potential against various types of cancer.[1] The molecule's unique structure, a sesquiterpenoid featuring a 1,2,4-trioxane ring, is central to its pharmacological activity.[2] This *endo*-peroxide is crucial, as its cleavage produces reactive intermediates with cytotoxic properties.[3] Whereas the activation of the peroxide *via* Fe(II) has been extensively investigated, the activation by electromagnetic radiation stands out and is subject of intensive research. In the intramolecular activation, a covalently linked artemisinin–sensitizer dyad is irradiated, which has proven to be a more effective strategy than to activate it intermolecularly.[4]

Herein, xanthone carboxylic acid derivatives were established as versatile building blocks for the synthesis of novel xanthone–artemisinin dyads. Using this approach, a first dihydroartemisinin dyad was obtained and comprehensively characterized. Upon irradiation with λ = 350 nm, moderately fast peroxide rearrangement is observed while the xanthone chromophore remains intact. The resulting decomposition products resemble those of well described iron-mediated activation, indicating a similar radical-based mechanism. Building on these findings, several new xanthone–artemisinin dyads with modified linker structures were synthesized to systematically investigate the influence of linker length, flexibility, and chemical nature. The results highlight the tunability of photophysical properties within this compound class and underscore the potential of xanthone carboxylic acids as scaffolds for the design of light-responsive artemisinin systems.[5]

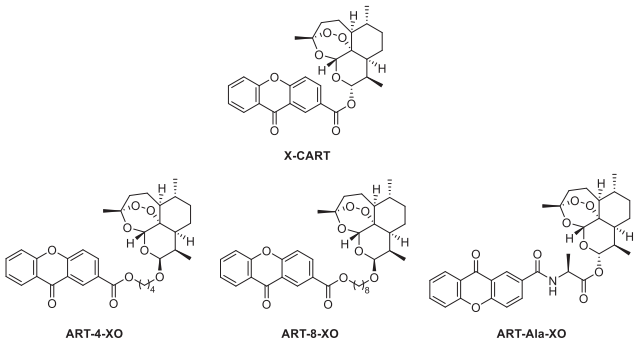

Figure 1: All synthesized and analyzed dyads.

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NMR-based Structure-Activity Relationship Studies of Antimicrobial Peptides

Sonja Bazhenova[1], Michael Quagliata[2], Joshua Grabeck[3], Philipp Holz[3], Kathrin König[1], Anna Maria Papini[2], Paolo Rovero[2], Ines Neundorf[3] and Daniel Friedrich[1]

[1] Department of Chemistry and Biochemistry, University of Cologne, Greinstr. 4, 50939 Cologne, Germany

[2] Interdepartmental Research Unit of Peptide and Protein Chemistry and Biology, Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia 13, I-50019 Sesto Fiorentino, Italy

[3] Institute of Biochemistry, University of Cologne, Zülpicherstr. 47a, 50674 Cologne, Germany

The rapid global rise of antibiotic resistance necessitates the development of new therapeutic strategies, with antimicrobial peptides (AMPs) representing a promising class of drug candidates. Building on our previous identification of two active AMPs, we performed an extended structure–activity relationship (SAR) analysis to dissect the relative contributions of hydrophobicity, secondary structure, and conformational constraint to antimicrobial efficacy.[1] Systematic amino acid substitutions were introduced into linear peptides to modulate hydrophobic surface area, while peptide cyclization was achieved *via* triazolyl bridges with varied position and ring strain. Antimicrobial activity assays revealed that increasing the hydrophobic surface in linear peptides consistently enhances antimicrobial potency. Likewise, in triazolyl-bridged peptides, increased ring strain generally correlates with improved activity, although both the position and orientation of the triazole bridge exert a pronounced influence on efficacy. NMR spectroscopy showed that linear peptides adopt predominantly random-coil conformations in aqueous solution, whereas N-terminal triazolyl cyclization induces partial α-helical structure. To rationalize these findings at the molecular level, we compared triazolyl-bridged peptides with their linear analogues using solution and micelle-bound NMR. Triazole-mediated prestructuring stabilizes a well-defined α-helix and promotes amphipathic surface organisation, characterised by spatial segregation of hydrophobic residues and a contiguous positively charged surface. Alanine scanning identified arginine residues at positions 3 and 7 and asparagine 11 as key contributors to antimicrobial activity, while lysine substitutions were less impactful. Micelle-bound structures further suggest that arginine 3 and asparagine 11 are directly involved in membrane interaction. Collectively, our results demonstrate that while α-helical preorganization and amphipathic enhance antimicrobial activity, the dominant driving force remains the extent and distribution of hydrophobic surface area. Fine-tuning hydrophobicity and conformational constraint through targeted substitutions and triazolyl cyclization emerges as an effective strategy for optimizing AMP activity.

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Removal of some heavy metals (Cu, Cd, Cr) by natural adsorbents

Sebnem D. Arıcı[1], Sevgi Kocaoba[1]

[1] *Yıldız Technical University, Faculty of Art and Science. Department of Chemistry, İstanbul, Türkiye*

Population growth, water scarcity and misuse, industrial growth, and the increasing amount of toxic heavy metals and other pollutants released into water resources are contributing to the growing demand for wastewater treatment on a global scale. One innovative water treatment technology is the adsorptive removal of heavy metals through the application of natural and waste-derived adsorbents.[1,2]

Heavy metals originating from various industrial facilities, agricultural areas, and household waste leave residues in food, entering the food chain and causing various diseases in humans and animals.[3]

This study investigated the removal conditions of Cu, Cd, and Cr heavy metals from environmental wastewater using natural wastes (pomegranate peel and peanut shell) and modified biochar. First, these fruit peels were dried and ground into ash. Their sizes were made uniform by sieving. Parameters such as adsorbent amount, pH, concentration, and stirring time were investigated to ensure suitable adsorption conditions.

The results obtained show that natural and sustainable materials can offer effective alternatives for heavy metal removal. The results obtained are consistent with those obtained in previous adsorption studies with similar materials.[4,5,6]

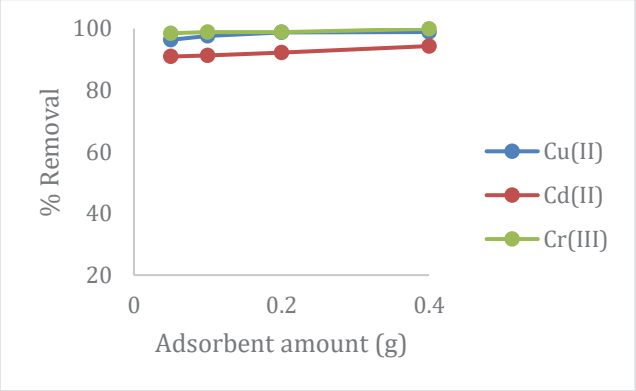

Figure 1: Removal percentages of Cu(II), Cr(III) and Cd(II) in peanut adsorption depending on adsorbent amount

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Faster grain-boundary diffusion with a higher activation enthalpy than bulk diffusion in ionic space-charge layers

Timon Kielgas,[1] Roger A. De Souza,[1]

[1] *RWTH Aachen University, Institute of Physical Chemistry, Aachen, Germany*

Faster diffusion of cations along grain boundaries is reported in the literature for a variety of acceptor-doped ABO_3 perovskite-type oxides. The ratio r of the activation enthalpy of grain-boundary diffusion (ΔH^{gb}) to the activation enthalpy of bulk diffusion (ΔH^{b}) is seen experimentally to lie in the range $0.7 < r = \Delta H^{gb} / \Delta H^{b} < 1.3$, albeit with substantial errors. In a previous publication [2] it was shown through a set of continuum simulations that cation-vacancy accumulation within negative space-charge layers at grain boundaries in acceptor-doped perovskites will give rise to faster grain-boundary diffusion of cations, with the associated values of r approaching but not exceeding unity. In the present study, we demonstrate by means of continuum simulations that under certain conditions $r > 1$ is achievable for faster cation diffusion along grain boundaries in an acceptor-doped perovskite ceramic. Diffusion profiles for a two-dimensional bicrystal geometry are obtained by solving, first, Poisson's equation, and subsequently, the diffusion equation. The specific case we consider is cation migration occurring by two related mechanisms, by isolated cation vacancies and by defect associates of cation and anion vacancies; the electric potential within the space-charge layers shifts the association equilibrium so that associate diffusion dominates in the bulk whereas isolated vacancy diffusion dominates within the space-charge layers.

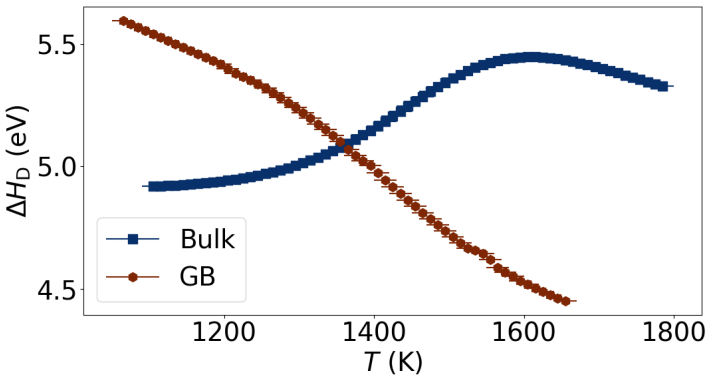

Figure 1: Activation enthalpy for diffusion as a function of temperature comparing diffusion in the bulk to the grain boundary. Towards lower temperatures, ΔH_D for the grain boundary strongly exceeds the bulk.

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Uv curable flame retardant paint coating

Nilsu Savaş[1] Tarık Eren[1]

[1]*Yildiz Technical University, Faculty of Art and Science*
Chemistry Department Istanbul,Turkiye

Flame retardancy is an essential quality for the performance and safety of textile materials used in everyday and industrial settings.[4] The primary objective of this study was to develop and implement an efficient UV curable flame retardant coating method on textile surfaces using phosphonate based additives.[1,2] Alendronate and glyphosate were chosen as flame retardants and reacted with ACOM (3-(acryloyloxy)-2-hydroxypropyl methacrylate) to yield reactive complexes.[1] These complexes were incorporated into a blank UV curable resin system containing a photoinitiator (DMPA).[3]

Cotton fabrics were coated using the dip coating technique and cured via UV irradiation in a reactor.[3] To assess system stability and success, the formulations precipitation behavior, solubility analysis, TLC, and FTIR spectroscopy characterizations were carried out. Flammability testing demonstrated that the alendronate based NS1 1 formulation was significantly more resistant to flames compared to the glyphosate based (NS2 2) samples.[2,4] Notably, NS1 1 treated fabrics successfully resisted ignition for 5 seconds upon exposure to an open flame at a distance of 5 cm. Among all studied samples, the NS1 1 formulation showed the most excellent thermal stability, coating durability, and flame retarding performance.[1,2,4] These findings demonstrate that alendronate based UV curable formulations show excellent potential as effective flame retardant coatings for textiles.



Figure 1: Flammability test image of cotton textile coated with alendronate-based UV-curable formulation.

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DNA-guided assembly of a Triplet-Triplet Annihilation Upconversion System

Sophie Lüggert,[1] Aiman Rauf,[2] Paul van Loosdrecht,[2] Stephanie Kath-Schorr[1]

[1] *University of Cologne, Institute of Organic Chemistry, Cologne, Germany*
[2] *University of Cologne, II. Physical Institute, Cologne, Germany*

Enhancing the efficiency of photovoltaic devices is a longstanding challenge, as conventional silicon-based solar cells cannot fully exploit the solar spectrum. Photon upconversion offers a promising approach to address this issue by converting low-energy photons into higher-energy photons that can be utilized by the silicon semiconductor.

Among various upconversion mechanisms, triplet–triplet annihilation (TTA), which relies on the interaction of sensitizer and annihilator chromophores, is especially attractive for this application, because it operates efficiently under low-light conditions. The efficiency of this process is highly sensitive to the distance and orientation of the chromophores, highlighting the need for self-assembly strategies that provide precise nanoscale organization.[1]

Here, we present a modular DNA-based self-assembly platform that enables the programmable organization of sensitizer and annihilator chromophores with nanometer precision. Using CuAAC chemistry, chromophores are covalently attached to oligonucleotides, and sequence-specific hybridization is employed to assemble discrete, well-defined dye aggregates of controlled size and composition. As a proof of concept, assemblies based on the well-established diphenylanthracene (DPA) / Pd-tetraphenylporphyrin (PdTPP) TTA-UC system are realized. Exciton dynamics in these assemblies shall be studied using transient optical spectroscopy to relate triplet energy transfer and triplet annihilation efficiency to the assembled chromophore arrangement.

This study aims to contribute to the self-assembly of triplet–triplet annihilation upconversion systems while highlighting DNA as a versatile platform for the organization of photonic materials.

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Accelerator produced ^{99m}Tc for medical applications: Technical and chemical optimizations and comparison with conventional Al_2O_3 generator systems

Marco Michel[1], Celina Sander[1], Diana Blaščanin[1], Bernd Neumaier[2], Klaus Eberhardt[3], Erik Strub[1]

[1]*University of Cologne, Faculty of Mathematics and Natural Sciences, Division of Nuclear Chemistry, Zülpicher Straße 45, Cologne, Germany*

[2]*Forschungszentrum Jülich GmbH, Institute of Neuroscience and Medicine – Nuclear Chemistry (INM-5), Jülich, Germany*

[3]*Johannes Gutenberg University Mainz, Research Reactor TRIGA Mainz, Fritz Strassmann Weg 2, Mainz, Germany*

The generation of ^{99m}Tc and its parent nuclide ^{99}Mo by means of various accelerator reactions has been heavily investigated in the last 10-20 years to find alternative production methods for ^{99}Mo as a parent of ^{99m}Tc.[1,2] ^{99}Mo is typically produced in nuclear reactors with a high-specific-activity (HSA). Owing to recent supply shortages efforts to find alternative sources for ^{99}Mo have intensified. One promising approach is neutron activation of ^{98}Mo, which yields low-specific-activity (LSA) ^{99}Mo. Since conventional Al_2O_3-based ^{99}Mo/^{99m}Tc generators are designed for HSA ^{99}Mo, modifications are required the application of LSA ^{99}Mo. Our experiments are based on the utilization of the planned 'High Brilliance Source System' (HBS) accelerator at the Forschungszentrum Jülich in Germany for neutron activation. We want to evaluate the feasibility of modifying conventional Al_2O_3-based ^{99}Mo/^{99m}Tc generators for use with LSA ^{99}Mo.[3] Key modifications included variations of the amount of Al_2O_3 on the column, the type of Al_2O_3 and elution volume for ^{99m}Tc to enhance ^{99}Mo adsorption and ^{99m}Tc elution efficiency. Further experiments using y-Al_2O_3 as a column material showed an increase in adsorption capacity for ^{99}Mo. The performance of the modified system was compared with that of a conventional clinical generator. Preliminary results indicate that its applicability as a clinically used Mo/Tc nuclide generator can be achieved, requiring only minor modifications for effective utilization of LSA ^{99}Mo.[4]

Acknowledgements:

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Unsymmetrical Anthracene Platforms for Oxygen Reservoir Applications

Finn Sobanja,[1] Vanessa Barth,[1] Henning J. Jessen[1]

[1]*Albert-Ludwigs-Universität, Institute of Organic Chemistry, Freiburg i. Brg., Germany*

Anthracene derivatives that reversibly store singlet oxygen ($^1O_2$) offer attractive opportunities for medical and pneumatic applications, as they enable controlled oxygen release without the need for an external photosensitizer. In this work, a synthetic strategy for **unsymmetrically substituted anthracene platforms**, combining a 9-meta-pyridyl and a 10-para-pyridylethynyl substituent, was developed and optimized.

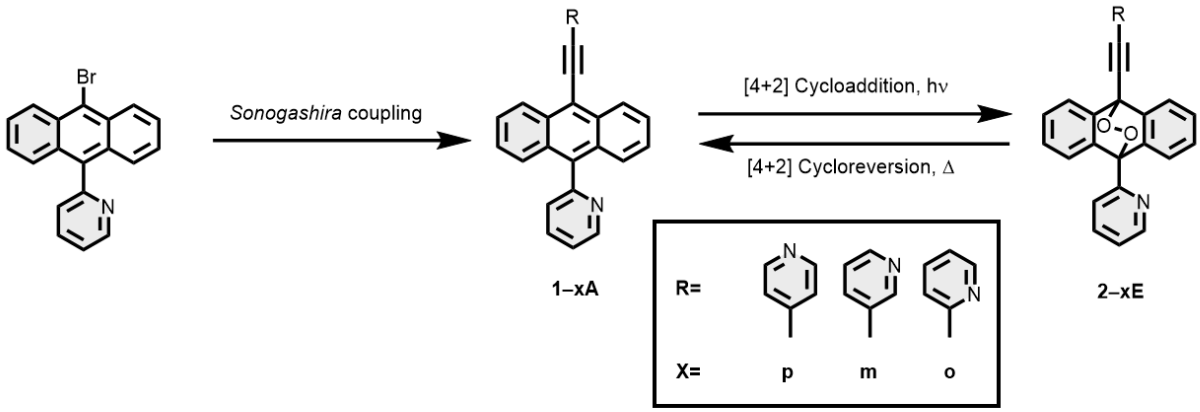

Figure 1. General scheme of the reactions conducted on the different anthracene platforms.

One novel anthracene platform (**1–pA**) was fully characterized and evaluated for its potential use in pneumatic systems. The investigated compound exhibits pronounced self-sensitizing behaviour, enabling efficient photooxygenation without added sensitizers. Kinetic studies reveal photooxidation rate constants that are an order of magnitude higher than those reported for comparable symmetric anthracene systems, indicating that self s-sensitizing accelerates $^1O_2$ addition.[1] Preliminary thermolysis experiments demonstrate clean and reversible release of singlet oxygen from the corresponding endoperoxides, highlighting the suitability of these systems as self-contained $^1O_2$ reservoirs.[2]

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Assessing Environmental Impacts of Multi-Step Synthetic Protocols in Material Sciences

Laura Plein,[1] Alexander Schommer,[2] Florian Dietrich,[1,2] Moritz Gutsch,[2] Heike Klesper,[1] Kevin Schuller,[1] Lars Jahnke,[2] Jens Leker,[2,3] Klaus Meerholz[1*]

[1] *University of Cologne, Institute for Light and Matter, Cologne, Germany*
[2] *University of Münster, Institute of Business Chemistry, Münster, Germany*
[3] *Forschungszentrum Jülich GmbH, Helmholtz Institut Münster, IEK-12, Münster, Germany*

Environmental awareness is increasing worldwide, driven by e.g. the climate change. Scientists are requested to research on “greener” materials to slow down or even reduce these issues. The development of novel materials, especially at an early-stage, shows high leverage and should go hand in hand with life cycle assessment (LCA) to monitor the environmental impacts. However, often LCAs consider only a few impact categories risking to overlook others or struggle with comparability since impact categories have different physical units.

Therefore, we introduce the Environmental Synthesis Radar (ESR) as formalism to systematically evaluate the environmental impacts of multi-step chemical synthesis routes considering 18 normalized midpoint impact categories. The validity of the ESR formalism is demonstrated for cathode materials in secondary batteries. We benchmark an emerging organic cathode material based on tris-(p-methoxy)-phenylamines (TPA), synthesized on lab scale only, against lithiated nickel-manganese-cobalt oxide (NMC) as inorganic reference, which is produced on an industrial level.

The TPA synthesis suffers from many steps required, more chemicals involved, and lower yields, leading to a 5-7 times higher impact per kg compared to the inorganic reference NMC. ESR reveals bottlenecks in synthesis, which after improvement allowed lowering the environmental impact of TPA by up to 18%, rendering the factor 2.

Overall, ESR provides an easily accessible, broadly applicable and versatile tool for researchers to evaluate and improve the environmental performance in material sciences.

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Drug combination screen on Salmonella persisters in Macrophages identified synergistic drug interactions

Alexandra Tietze[1,2] and Ana Rita Brochado[1,2,3]

[1] Department of Microbiology, Biocenter, University of Würzburg, Würzburg, Germany
[2] Interfaculty Institute of Microbiology & Infection Medicine Tübingen (IMIT), University of Tübingen, Tübingen, Germany
[3]Cluster of Excellence 'Controlling Microbes to Fight Infections' (CMFI), University of Tübingen, Tübingen, Germany

Intracellular pathogens such as Salmonella pose a major challenge in the context of infectious diseases due to their ability to enter a persistent state, evading both host immunity and antibiotics. Understanding the interplay between pathogen survival strategies and innate immune responses, especially after pathogen internalization and establishment in the intracellular niche, is critical for developing new therapeutic approaches.

In this study, we developed a high-throughput screening approach to evaluate the effects of 3000 drug combinations on sustaining or aborting Salmonella Typhimurium infections within macrophages (Fig. 1). We simultaneously target the bacterium and the macrophage using a combination of antibiotics and immunomodulatory drugs to identify conditions that interfere with host-pathogen interactions well after Salmonella's establishment in the intracellular niche, thereby altering its intracellular survival. We used recovery time after antibiotic removal to quantify bacterial viability and post-treatment-stress effects at scale.

We identified multiple drug combinations that effectively modulate the Salmonella's recovery time, primarily synergistic effects causing recovering times significantly longer than expected based on the effect of the drugs alone. Importantly, we found several compounds, which targets have been previously reported to hamper Salmonella intracellular survival (e.g. ROS production), thereby legitimating of our approach. In addition, we found synergistic interactions involving compounds targeting host pathways for which there is no previous evidence of relevance to Salmonella persistence. We are currently pursuing in-depth exploration of these leads, which will unveil the molecular mechanism of this synergy on the bacterial and host sides, and potentially reveal novel pathogen survival strategies.

In the long term, we aim to investigate how pathogen- or host-cell-specific our findings are, which will hint towards the need for broad-spectrum or targeted therapies. These results demonstrate the power of systems biology to uncover critical molecular interactions in innate immunity and provide actionable insights for combating persistent bacterial infections.

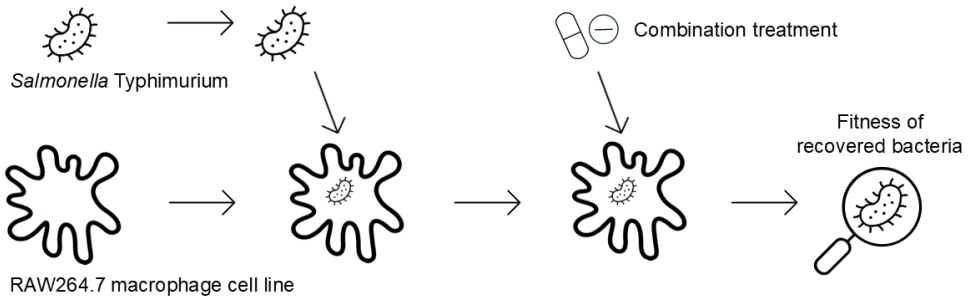

Figure 1: Schematic workflow of the infection screen.