Second Erlangen Symposium



Image: FAU/Georg Pöhlein



Book of Abstracts

June 18-20, 2023 Chemikum Erlangen, Germany





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Preface

The **Women in Science-2nd Erlangen Symposium** was organized over the last year by female doctoral students and postdoctoral researchers from the Department of Chemistry and Pharmacy at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU). First conceptualized in 2018, the main goal of this initiative is to tackle the underrepresentation of women in science by increasing the visibility of female researchers, establishing a global network, and fostering conversations among all genders on how we can achieve gender equality in science.

The symposium will host over 190 participants from eight countries and diverse fields, including organic chemistry, organometallic chemistry, and materials science, among others. Over the course of the event, distinguished female speakers will not only present their research findings, but also share their challenges and pathways toward success in academia and/or industry. The participants, especially young researchers, will have the opportunity to build new connections and collaborations, while gaining insights into career prospects. The program also includes eleven flash talks, thirty-three poster contributions and a "braindating" session. Additionally, dedicated time will be allocated for roundtable discussion to address gender inequality in work–life balance. Although our primary focus is on women in science, the symposium is open to everyone, irrespective of gender or status. Each symposium session or activity therefore aims to present scientific work and facilitate many fruitful discussions, encouraging male, female, and non-binary researchers to actively participate in the symposium.

We hope that the symposium will serve as a unique and inclusive platform for all participants and promote future collaborations. We wish you a pleasant stay in Erlangen!

WIS2023 Organizing Committee



WIS2023 Organizing Committee

Dr. Stefanie Klein

Dr. Ani Özcelik

Dr. M. Eugenia Pérez-Ojeda

Dr. Rachel Vykukal

Dr. Susanne Wintzheimer

Sara Li Deuso

Marie Freiberger

Swathi Krishna

Elena Mack

Hannah Stecher

Natalie Waleska-Wellnhofer

Taha El Sayed





General information

Conference Site:

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



Photo: Helen Hölzel

The 'Chemikum' building of FAU represents the ideal location for the symposium, housing several of FAU's chemistry departments under its roof. Fully equipped lecture halls ensure the realization of this event in a modern environment. It also offers ample room for the poster session, stimulating and inspiring further discussions.

Please see the following map of the Chemikum for details. All lectures will take place in the lecture hall **C1**. Coffee breaks, lunch, and the poster session will be in and around the **seminar room.** Both rooms are located on the ground floor.





Transportation

Airports:

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

Public Transport:

- Bus tickets can be purchased on the bus with cash or with debit/credit cards on the VGN app; train tickets can be purchased at one of the automatic machines at the station, on the VGN app, or the Deutsche Bahn (DB) app
- A single one-way trip within the Erlangen area, including to FAU's campus, costs 2.25€
- <u>From Nuremberg:</u> take the **VGN Bus 30** to the bus stop "Erlangen Süd" or a local train to the main Erlangen train station and one of the buses below
- <u>Train:</u> there are four train stations within Erlangen; the main train station is called "Erlangen Bahnstation" on Bahnhofplatz, which is considered city center
- o <u>Bus:</u> from main train station "Erlangen Bahnstation", the following buses depart regularly:
 - **Bus 287** direction "Sebaldussiedlung," stop at "Technische Fakultät", then approx. 5 min walk to Chemikum
 - **Bus 293** direction "Bruck Bahnhof", stop at "Sebaldussiedlung", then approx. 3 min walk to Chemikum
 - **Bus 295** direction "Tennenlohe", stop at "Erlangen Süd", then approx. 12 min walk to Chemikum



Please see the following sites and apps for current timetables, bus stop map at left, and bus stop designation symbol below.



www.vgn.de www.bahn.de

VGN app

DB app



Detailed Program

Sunday, June 18 th 2023		
12:00 - 14:00	Registration	
14:00 – 14:15	Opening Remarks by the Organizing Committee	
Chairperson - Swathi Krishna		
14:15 – 15:15	Keynote Lecture: Luisa De Cola, Universita di Milano	
	Responsive Organosilica Nanoparticles	
15:15 – 15:40	Invited Lecture: Danijela Gregurec, Friedrich-Alexander-Universität Erlangen- Nürnberg	
	Remotely Responsive Magnetic Nanomaterials for Neuromodulation	
15:40 – 15:50	Siow Woon Ng, Friedrich-Alexander-Universität Erlangen-Nürnberg	
	Ultrathin ALD Coatings on Complex Geometries for Sensing and Catalytic Applications	
15:50 – 16:30	Coffee Break – Discussion with Speakers	
Chairperson – Simon Hammann		
16:30 – 17:15	Invited Lecture: Jenny Zhang, University of Cambridge	
	Shooting for Sustainability (online)	
17:15 – 17:25	Jenny Schneider, Ludwig-Maximilians-Universität München	
	Photocatalysis as a Tool to Tackle Global Warming	
17:25 – 18:10	Invited Lecture: Sara Aldabe Bilmes, Universidad de Buenos Aires	
	The Challenge of Preparing Tailored Materials and Sharing Knowledge with the New Generations	
19:30 –	Speakers Dinner (invitation only)	
	Student Dinner at <i>Gaststätte mit Biergarten "Am Röthelheim</i> (Am Röthelheim 40, 91052 Erlangen) (self-pay)	



Monday, June 19 th 2023		
09:00 - 09:30	Welcome Addresses	
	Andreas Hirsch, Friedrich-Alexander-Universität Erlangen-Nürnberg	
	Lina Seitzl, Member of the Bundestag	
Chairperson - Dirk Guldi		
09:30 – 10:30	Keynote Lecture: Isabel Pastoriza-Santos, Universidade de Vigo	
	Synthesis and Applications of Plasmonic Nanoparticles	
10:30 – 10:50	Invited Lecture: Magda Luthay, Friedrich-Alexander-Universität Erlangen- Nürnberg	
	Bridging the Gender Gap: Women in Science and Academia	
10:50 – 11:15	Invited Lecture: Andrea Büttner, Friedrich-Alexander-Universität Erlangen- Nürnberg	
	Trust your Senses, Follow your Nose Why Comprehension of Bioeconomy has a lot to do with Perception	
11:15 – 12:00	Invited Lecture: Roberta Romano-Götsch, European Patent Office	
	Women's Participation in Inventive Activity	
12:00 – 13:00	Lunch Break	
Chairperson – Ir	ngrid Span	
13:00 – 13:45	Invited Lecture: Marika Schleberger, Universität Duisburg-Essen	
	From Surfaces Physics to Two-Dimensional Materials – and why you should not be afraid of Serendipity	
13:45 – 13:55	Marta Alcaraz, Universidad de Valencia	
	Colloidal Synthesis of 2D-Pnictogens: Antimonene and Bismuthene	
13:55 – 14:40	Invited Lecture: Paula Diaconescu, University of California, Los Angeles	
	Redox Switchable Ring Opening Copolymerization	
14:40 – 14:50	Lisa Gravogl, Friedrich-Alexander-Universität Erlangen-Nürnberg	
	A Phenolate-Carbene Supported High-Valent Fe–O Intermediate Derived From Dioxygen	
14:50 – 16:10	Coffee Break with Roundtable Discussions	
	Marcus Halik, Friedrich-Alexander-Universität Erlangen-Nürnberg	
	Susanne Wintzheimer, Friedrich-Alexander-Universität Erlangen-Nürnberg	



Chairperson – Marcus Halik		
16:10 – 16:55	Invited Lecture: Sophie Beeren, Danmarks Tekniske Universitet	
	Enzyme-Mediated Dynamic Combinatorial Chemistry with Cyclodextrins	
16:55 – 17:05	Asli Can Karaca, Istanbul Teknik Üniversitesi	
	Recent Advances in the Modification of Surface Characteristics and Functionality of Plant Proteins	
17:05 – 17:15	Theresa Maria Schichtl, Friedrich-Alexander-Universität Erlangen-Nürnberg	
	Effect of Vitamin B_6 on the Formation of Non-Enzymatic Protein Modifications in Heat-Treated Whey	
17:15 – 19:00	Poster Session	
19:00 –	Barbecue (outside the Chemikum at the main entrance) and Scientific Discussions	

Tuesday, June 20 th 2023		
Chairperson – Hannah Zenker		
09:00 - 09:45	Invited Lecture: Derya Baran, King Abdullah University of Science and Technology	
00.45 00.55		
09:45 - 09:55	LISA M. S. Stiegier, Friedrich-Alexander-Universität Erlangen-Nurnberg	
	Characterization of Complex Colloidal Nanomaterials by Analytical Ultracentrifugation (AUC)	
09:55 – 10:40	Invited Lecture: Marta Liras, Instituto IMDEA Energía	
	Conjugated Porous Polymer and Hybrid thereof Ground-Breaking Materials for Solar Energy Conversion	
10:40 – 11:50	Coffee Break with Braindating	
Chairperson – Hannah Smith		
11:50 – 12:00	Caterina Bellatreccia, Università di Bologna	
	CuInS2 Nanocrystals for Solar-Driven Oxidation of Redox Mediators	



12:00 – 12:10	Giovanni M. Beneventi, Friedrich-Alexander-Universität Erlangen-Nürnberg
	On the Rich Photophysical Properties of Nitrogen-Containing Molecular
	Nanographenes and their Coordination Compounds
12:10 – 12:20	Hemlata Agarwala, Technische Universität München
	Alternating Substrate-Ligand Coordination Provides a Lower Energy C-O Bond Cleavage Pathway for Electrochemically Driven Catalytic CO ₂ Reduction
12:20 – 13:35	Lunch Break
Chairperson – Svetlana Tsogoeva	
13:35 – 14:20	Invited Lecture: Rajyashree Sundaram, Huawei Nuremberg Research Center
	A Journey across the World for Nano(carbon)materials
14:20 – 14:30	Sophie R. Thomas, Technische Universität München
	Water-Soluble Gold Nanoparticles Stabilized by N-Heterocyclic Carbenes for Applications in Catalysis and Medicine
14:30 – 14:55	Invited Lecture: Sabine Maier, Friedrich-Alexander-Universität Erlangen- Nürnberg
	On-Surface Synthesis: a Bottom-Up Strategy to Low-Dimensional Carbon- Structures
14:55 – 15:20	Award Ceremony, Closing Remarks and Announcement of Women in Science Symposium 2024

Keynote Speakers

Prof. Luisa De Cola



Università di Milano Mario Negri Institute for Pharmacological Research

Prof. Luisa De Cola is working in two main research areas: a) luminescent and electro-luminescent materials for optical and electroluminescent devices; b) nanomaterials and soft matrices for imaging, diagnostics and therapy.

Website for further information: www.unimi.it/en/ugov/person/luisa-decola

Prof. Isabel Pastoriza-Santos

Universidad de Vigo Faculty of Chemistry



Prof. Isabel Pastoriza-Santos' research interest involves the synthesis, assembly and surface modification of nanoparticles with unique properties as well as development of (multi)functional nanostructured materials and tools with applicability in nanoplasmonics, (bio)sensing, catalysis and biomedicine.

Website for further information: www.coloides.webs.uvigo.es/portfolio/isabel-pastorizasantos/



Invited Speakers

Prof. Derya Baran



King Abdullah University of Science and Technology Material Science and Engineering

Prof. Derya Baran's research interests lie in the area of solution processable organic/hybrid soft materials, which possess a viable platform for printed, large area, stretchable and wearable electronics that can be used as solar cells, smart windows, OFETs, thermoelectrics, sensors and bio-electronics.

Website for further information: www.kaust.edu.sa/en/study/faculty/derya-baran

Prof. Sophie Beeren



Technical University of Denmark Department of Chemistry

Prof. Sophie Beeren expertise concerns supramolecular chemistry, physical organic chemistry, chemical biology, molecular recognition, carbohydrate enzymology, organic synthesis, and molecular design.

Website for further information: www.kemi.dtu.dk/sophiebeeren

Prof. Sara Aldabe Bilmes



Universidad de Buenos Aires Facultad de Ciencias Exactas y Naturales

Prof. Sara Aldabe Bilmes' research is targeted to understand process at solid-liquid interfaces that are relevant for decontamination. This includes the soft synthesis of nanomaterials and nanostructures with controlled structure, porosity and defects that can host molecules, nanoparticles and living cells.

Website for further information: www.qi.fcen.uba.ar/academicos/integrantes/ profesores?id=14

Prof. Andrea Büttner



Friedrich-Alexander-Universität Erlangen-Nürnberg Department of Chemistry and Pharmacy; Fraunhofer IVV

Prof. Andrea Büttner focuses on improving and maintaining food and product quality, analysis of aroma and non-food smell, impurity and contaminant analysis, and developing analytics and diagnostics in networked and intelligent systems, to ensure the highest product quality and consumer acceptance. She emphasizes sustainable and resource-saving management as well as product safety and consumer protection.

Website for further information: www.chemistry.nat.fau.eu/aroma-smell-research/ curriculum-vitae

Prof. Paula L. Diaconescu



University of California, Los Angeles Chemistry & Biochemistry

Dr. Paula Diaconescu's current research efforts focus on the design of reactive metal complexes with applications to small molecule activation, organic synthesis, and polymer formation.

Website for further information: www.chemistry.ucla.edu/directory/diaconescu-paula-l/

Prof. Danijela Gregurec



Friedrich-Alexander-Universität Erlangen-Nürnberg Department of Chemistry and Pharmacy

Prof. Danijela Gregurec's research is multidisciplinary and spans from engineering of tools and interfaces for cellular control and elucidating biophysical interfacial mechanisms to the interrogation of neuronal signaling. Her group is developing intelligent nanomaterials for wireless sensing and actuating of neuronal activity to repair or replace lost biological functions.

Website for further information: www.chemistry.nat.fau.eu/aroma-smell-research/prof-drdanijela-gregurec/

Dr. Marta Liras



IMDEA Energy

Dr. Marta Liras is using her expertise, specially in polymer science, to develop new technologies in the energy field such as the design of multifunctional hybrid photo(electro)catalyst as well as the design of energy storage systems.

Website for further information: www.energia.imdea.org/investigacion-unidades-deprocesos-fotoactivados/

Dr. Magda Luthay



Friedrich-Alexander-Universität Erlangen-Nürnberg Office for Equality and Diversity

Dr. Magda Luthay holds a degree in Middle Eastern Studies and Modern History from FAU. Her doctoral thesis deals with the Implementation of the United Nations Convention on the Elimination of all forms of Discrimination against Women (CEDAW) in the United Arab Emirates. In addition, she has a long-term working experience in the media business as a journalist.

Website for further information: www.gender-und-diversity.fau.de

Prof. Sabine Maier



Friedrich-Alexander-Universität Erlangen-Nürnberg Department of Physics

Prof. Sabine Maier's research focuses on surfacesupported molecular nanostructures and two-dimensional materials using high-resolution scanning probe microscopy and spectroscopy. Her group studies singlemolecule processes, self-assembly of supramolecular structures, and on-surface synthesis of novel carbonbased materials.

Website for further information: www.spm.nat.fau.de/

European Patent Office

Chief Sustainability

Dr. Roberta Romano-Götsch



Dr. Roberta Romano-Götsch serves as Chief Sustainability Officer since January 2022. Prior to that she served as Chief Operating Officer of the sector Healthcare, Biotechnology and Chemistry, and earlier in Mobility and Mechatronics, responsible for leading 1600 patent examiners in Munich, Berlin and The Hague. She obtained a PhD in organic chemistry from TU Munich.

Website for further information: www.epo.org/index.html

Prof. Marika Schleberger



Universität Duisburg-Essen Faculty of Physics and CENIDE

Prof. Marika Schleberger's research expertise is 2Dmaterials (synthesis, properties, tailoring, devices, and applications); ion-solid interaction; surface science; scanning probe and correlative microscopy. She looks forward to the opportunities and challenges that AI and machine learning will open up in her research field and in teaching.

Website for further information: www.uni-due.de/physik/schleberger

Dr. Rajyashree Sundaram



Huawei Nuremberg Research Center Power Conversion Technology Laboratory

Dr. Rajyashree Sundaram's research experience is on manufacture and application-development of nanocarbon-based materials, including composites. One area she is focusing on currently is research and application development of thermal management materials for high power electronics.

Website for further information: www.linkedin.com/in/rajyashree-sundaram

Dr. Jenny Zhang



University of Cambridge Yusuf Hamied Department of Chemistry

Dr. Jenny Zhang's research aims to develop smart biohybrid approaches that can serve as tools to understand the bioenergetics of complex biological systems and as a platform to launch new biotechnologies to address a range of societal needs (including for renewable energy generation, carbon capture, precision farming, environmental sensing, and medicine).

Website for further information: www.ch.cam.ac.uk/person/jz366

Abstracts



Keynote Speakers

Responsive Organosilica Nanoparticles

Luisa De Cola¹

¹Institute of Pharmacological Research Mario Negri, and University of Milano, Via C. Golgi 19, 20124 Milano, Italy luisa.decola@unimi.it

The development of smart nanoparticles (NPs) that encode responsive features in the structural framework promises to extend the applications of NP-based drugs, vaccines, and diagnostic tools. We have developed nanoparticles able to break on demand and proven their use as drug delivery systems for aggressive tumors.[1] In particular we have used a special morphology, a nanocage structure of only 20 nm that is able to escape macrophage uptake [2] and to stabilize species out of equilibrium for days[3]

More recently, through a nature-inspired approach that combines the programmability of nucleic acid interactions and sol-gel chemistry. In the contribution the incorporation of synthetic nucleic acids and analogs as constitutive components of the organosilica NP structures will be discussed. In particular are illustrated nanomaterials containing single-stranded nucleic acids that are covalently embedded in the silica networks as well as combining the supramolecular programmability of nucleic acid (NA) interactions with sol-gel chemistry the first example of supramolecular silica. This approach allows us to create dynamic bridging units of nucleic acids implemented in a silica-based scaffold. In addition the implementation of a functional NA such as an aptamer, as silica connection, can lead to a specific recognition of ATP molecules.

References

- [1] M. Sancho-Albero, et al. Adv. Health. Mater. 2023, https://doi.org/10.1002/adhm.202202932
- [2] L. Talamini, et al. ACS Nano 2021, 15, 9701–9716
- [3] P. Picchetti, et al. J. Am. Chem. Soc. 2021, 143, 7681-7687
- [4] P. Picchetti, et al. J. Am. Chem. Soc. 2023, under revision.



Synthesis and Applications of Plasmonic Nanoparticles

Isabel Pastoriza-Santos¹

¹CINBIO, Universidade de Vigo, Lagoas Marcosende, 36310 Vigo, Spain pastoriza@uvigo.gal

The novel field of Nanoplasmonics focuses on the manipulation of light using materials with significantly smaller sizes than the radiation wavelength. This is typically achieved using nanostructured metals since they can very efficiently absorb and scatter light due to their ability to support coherent oscillations of free (conduction) electrons. The great development of nanoplasmonics is based on fine control over the composition and morphology of nanostructured metals. Particularly, wet-chemical methods have the advantage of simplicity and large-scale production, while offering several parameters that could determine the final particle morphology and surface properties, which is essential for further applications. This seminar will provide an overview of the optical properties of metal nanoparticles as well as the synthetic strategies to achieve size and shape control. Besides, I will show recent developments of the FunNanoBio Group in the Nanoplasmonic field with special emphasis on plasmonic nanostructures for (bio)sensing based on surface-enhanced Raman scattering and localized surface plasmon resonance and catalysis.



Invited Speakers



Chasing Answers: A chemist's material journey to make a difference

Derya Baran¹

¹King Abdullah University of Science and Technology (KAUST), Material Science and Engineering Program (MSE), KAUST Solar Center (KSC), 23955, Thuwal, Saudi Arabia derya.baran@kaust.edu.sa

Every scientific discovery starts with a question. Then, it is a journey chasing the answer/s. Life is not any different. Asking the right question is very important and to learn where to look for the answer and which tools you need to use. In this talk, I will share my journey chasing my own answers. I will share how I overcome biases and hurdles, what motivated me to science and academic life (well then combined with an entrepreneurial life) and will share my research passion which is solution processed energy conversion materials and devices.

The need for big data that the internet of things (IoT) has created in recent years has turned the focus on integrating the human body in the quest to understand it better, and in turn use such information for detection and prevention of harmful conditions. Applications in which continuous and uninterrupted operation is required, or where the use of external power sources may be challenging demands the use of self-powered autonomous systems. Organic photovoltaic devices are flexible, lightweight, and soft, capable of interacting with the human body and its mechanical demands. Their processability from solutions permits their adaptation to versatile fabrication techniques such as spin coating, roll-to-roll coating and inkjet printing, with benefits including low material usage and freedom of design. In this talk, I will present how organic photovoltaics can be utilized in printed electronics as energy harvesting devices.



Enzyme-mediated dynamic combinatorial chemistry with cyclodextrins

Sophie R. Beeren¹

¹Department of Chemistry, Technical University of Denmark, Kemitorvet Building 207 Kongens Lyngby 2800 Denmark sopbee@kemi.dtu.dk

Biomolecular templates define the outcomes of enzymatic reactions in some of the most fundamental of biological processes, such as DNA replication, transcription and translation. In synthetic chemistry, molecular templates have enabled the synthesis of highly complex molecular architectures and interlocked structures. With *Enzyme-Mediated Dynamic Combinatorial Chemistry*¹ we explore the possibility to use synthetic templates to direct enzymatic reactions and obtain alternative products to those generated in Nature.

Cyclodextrins (CDs) are macrocycles formed from α -1,4-linked glucopyranose units, and the cyclodextrins with 6, 7, and 8 glucose units (α - β - and γ -CD) are industrially important hosts for the encapsulation of hydrophobic molecules, such as pharmaceuticals, flavours and aromas. While these cyclic oligosaccharides are usually considered as stable, static molecules, we can generate dynamic mixtures of interconverting cyclodextrins by the action of *cyclodextrin glucanotransferase* (CGTase), which catalyses reversible transglycosylation.² When the system is dynamic, it can be manipulated via supramolecular interactions with artificial template molecules to alter the product distribution. We use templates to direct the selective synthesis of specific cyclodextrins, including modified cyclodextrins² and unusual large-ring cyclodextrins with more than 8 glucose units.³ By using stimuli-responsive templates, we can also control the outcome of this enzymatic reaction by means of external stimuli, such as light.⁴



Figure 1. Cyclodextrin glucanotransferase (CGTase) converts cyclodextrins from static molecules into a dynamic mixture of interconverting cyclic and linear oligosaccharides. Templates (guest molecules) can be added to control which cyclodextrin products are formed.

References

[1] Larsen, D.; Beeren, S. R., Chem. Sci., 2019, 10, 9981–9987.

[2] Larsen, D.; Ferreira, M.; Tilloy, S.; Monflier, E.; Beeren, S. R., *Chem. Commun.*, **2022**, *58*, 2287–2290.

[3] Erichsen, A.; Peters, G. H. J; Beeren, S. R., J. Am. Chem. Soc., 2023, 145, 4882–4891.

[4] Yang, S.; Larsen, D.; Pellegrini, M.; Meier, S.; Mierke, D. F.; Beeren, S. R.; Aprahamian, I., *Chem.*, **2021**, *7*, 2190–2200.



The challenge of preparing tailored materials and sharing knowledge with the new generations

Sara A. Bilmes¹

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We live in a world avid for new materials, in a consumer society where science and technology have been at the service of producing more and better products since the industrial revolution. This voracity has made us neglect the planet we inhabit and today we have a serious problem of polluted water, air and soil that affect the life of all the species that populate the Earth. The art of chemistry has, until the end of the 20th century, focused on extracting natural resources and producing materials by privileging yield and conservation of process, without considering the impact of by-products.

Sol-gel processes are a mild synthetic approach -*Chimie douce*- that mimic the abilities of living organisms to synthesize inorganic compounds (carbonates, silicates, phosphates) at room temperature and with defined functionalities. Within this approach schematized in Figure 1 we have synthesized metallic oxides oriented to environmental prevention and remediation. Our motivation is to understand chemistry at the nanoscale to achieve a rational design of materials.

In this talk, I will present some examples of synthesis of TiO_2 photocatalysts, SiO_2 hydrogels for encapsulating microorganisms, and mesoporous oxides with tailored pore distribution. This controlled synthesis allowed us to contribute to unravel the complexity involved in the physical chemistry of interfaces in confined media.

In addition, I will discuss new approaches for sharing our scientific knowledge with students, opposite to traditional teaching, with aim to introduce the new generations in the world of complexity.



Figure 1. sol-gel integrative chemistry for building materials with targeted applications



Trust your senses, follow your nose... Why comprehension of bioeconomy has a lot to do with perception

Andrea Buettner^{1,2}

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Our world is changing. The way we live and do business is constantly being questioned, and the use of our resources is increasingly being viewed from the perspective of crisis scenarios. The bioeconomy in particular, i.e. the use of biogenic, renewable raw materials and thus the management of our basic resources of water, earth and air, is in the spotlight. What is required are fundamentally new processes and technologies for the utilization and management of soil, water, and air - accompanied by new types of products that are supposed to meet the demands of sustainability, but also of resilient and sovereign supply and recyclability, ideally without giving the impression of abandonment and scarcity. But how is this change perceived and ultimately accepted? What role does sensory research play in this? And how can we facilitate and accompany this transformation with the help of sensory research? In the end, people have to like what the future brings... The lecture offers examples of how chemistry, technology and sensory sciences can jointly show new ways, in interaction with numerous other disciplines, and foster partnerships between institutions, disciplines and project landscapes – for a joint mission [1,2,3].

References

[1] https://www.chemistry.nat.fau.eu/aroma-smell-research/sensory-sciences-lecture-series/

[2] https://www.food.fraunhofer.de/

[3] https://www.fraunhofer.de/en/research/fraunhofer-strategic-research-fields/bioeconomy.html



Redox switchable ring opening copolymerization

Paula L. Diaconescu¹

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Switchable polymerization processes have received increased attention because they hold the promise of mimicking the selectivity exhibited by natural systems.¹⁻³ We are studying a chemical method to shuttle between two catalyst states, by switching the oxidation state of iron in ligands containing a ferrocene backbone. This idea is applied to the ring opening polymerization of cyclic esters/ethers catalyzed by transition metal complexes with the goal of forming biodegradable copolymers.



References

1. Deng, S.; Jolly, B. J.; Wilkes, J. R.; Mu, Y.; Byers, J. A.; Do, L. H.; Miller, A. J. M.; Wang, D.; Liu, C.; Diaconescu, P. L., Spatiotemporal control for integrated catalysis. *Nat. Rev. Methods Primers* **2023**, *3*, 28.

2. Lai, A.; Hern, Z. C.; Shen, Y.; Dai, R.; Diaconescu, P. L., 9.07 - Metal Complexes for Redox Switching and Control of Reactivity. In *Comprehensive Coordination Chemistry III*, Constable, E. C.; Parkin, G.; Que Jr, L., Eds. Elsevier: Oxford, 2021; pp 155-180.

3. Wei, J.; Diaconescu, P. L., Redox-switchable Ring-opening Polymerization with Ferrocene Derivatives. *Acc. Chem. Res.* **2019**, *52* (2), 415-424.



Remotely responsive magnetic nanomaterials for neuromodulation

Danijela Gregurec¹

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The emergence of a new era in neuromodulation is led by the intriguing potential of functional materials to replace or control neural activity. Wireless neuromodulation schemes can replace invasive brain surgeries and enable cell-precise neuronal control. Intrinsic properties of magnetic nanomaterials coupled to external magnetic fields (MFs) have recently permitted deep brain stimulation and relief of Parkinsonian symptoms in rodents trough hysteretic heating of magnetic isotropic nanoparticles acting on chemosensory ion channels in highfrequency alternating MFs[1]. More energy efficient approach for neuronal modulation with high spatiotemporal precision is based on development of novel class of anisotropic magnetic nanomaterials, magnetite nanodiscs (MNDs). These MNDs exhibit a characteristic vortex alignment of magnetic spins with zero net magnetization in the absence of external MFs. When the MF is applied, magnetization transitions from vortex to in plane allowing for the exertion of the torques on the pN scale, sufficient to activate mechanosensitive ion channels in cell membranes. We have shown remote control of activity in sensory neurons with weak (7-26 mT), slow-varying (1-5 Hz) magnetic fields coupled to MNDs. When coupled to mechanosensory ion channels, such as Transient receptor potential vanilloid family member 4 (TRPV4), a cell/protein- specific modulation is achieved[2].

Consistent with geometry and chemical composition, MNDs exhibit direction-dependent hysteresis loops and with high specific loss power (SLP) at kHz frequencies and low concentrations. Targeted activation of heat gated channels is thus permitted at high frequency alternating MFs. Therefore, MNDs allow for simultaneous stimulation of neurons by selectively activating mechanoreceptors at 1-5 Hz MFs, while heat dissipation and consequent activation of heat-gated ion channels is allowed at frequencies 75-150 kHz.



Figure 1. Remote selective activation of heat- and/or mechanosensitive neurons by switching between MF parameters

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Conjugated Porous Polymer and Hybrid thereof Ground-Breaking Materials for Solar Energy Conversion

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Solar energy conversion plays an important role in the transition to more sustainable energy technologies. Both demographic growth and industrialization leads to an increase in the consumption of solid fuels which the consequent planet temperature rise and appearance of associated environmental problems. Thus, the development of new technologies to storage renewables energy is a matter of importance in the transition to a greener energy pool. In this sense, artificial photosynthesis (AP), which convert CO₂, and water as raw materials by the action of solar energy in valued chemicals or fuels, could be an attractive solution. Here, the look for new materials able to produce solar fuels as efficient manner is a challenge. Conjugated (micro)porous polymers (CMPs or CPPs) as well as their crystalline analogs

Covalent Organic Framework (COFs) have appeared recently as alternative to inorganic semiconductor, metal oxides and chalcogenides, the typical photocatalyst used in AP.^[1]

In this talk, I am going to show our last result in the use of CPPs and COFs as well as hybrid thereof in AP processes such as hydrogen production from water and CO₂ photoreduction. The first design key is the choice of the main structural moiety, fundamental to determine their performance. Here, CPPs based on truxenes^[2], BODIPY^[3], BOPHY^[4] and phenanthrenequinone,^[5] will be

part

of

hybrid

as

Figure 1. Cartoon describing an AP system based on CPPs and IS

photocatalysis. The second key design is the nanostructuration of the polymer which lead to an improvement in the photocatalyst as well as allow the accessibility of thin films.^[6] Finally it will be discussed the effect of the crystallinity over these systems. On the other hand, the elucidation of the charge transfer mechanism is really important to explain the photocatalytic results, and also will be explained.

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Bridging the Gender Gap: Women in Science and Academia

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Political commitments to strengthen the presence, participation and progression of women in higher education have been made throughout the past few years on a national and local level.

At FAU a variety of approaches and measures have been successfully implemented in the past decade to foster gender equality in research by addressing the under-representation of women (e.g. in STEM fields) through a roadmap of activities and measures.

Despite the progress efforts are still needed to reduce the challenges female scientists are facing on their career path. In this context it is important to understand the factors contributing to these persisting inequalities.

So let's shed light on intrinsic as well as extrinsic factors which might contribute to the high dropout rate of women after their doctoral degree and let's discuss coping strategies to overcome obstacles.

How can we combat the following phenomenons: The Matilda Effect, the Impostor Syndrome, Gender Biases in Appointment Policies or the Glass Ceiling in academia?



FAU's Equality Strategy

Figure 1. FAU Strategies: Gender Equality Plan 2023-2027

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On-surface synthesis: a bottom-up strategy to low-dimensional carbon-structures

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On-surface synthesis via covalent coupling of adsorbed molecules on metal surfaces has attracted significant attention in recent years due to its potential to fabricate low-dimensional carbon materials with atomic precision. The bottom-up, atomically precise synthesis of carbon nanostructures enables the tailoring of their electronic properties at a molecular level. To understand and control the surface-chemistry-driven synthesis, many efforts have been made to design smart precursors, explore novel reaction schemes, and utilize templating effects from the substrate. Scanning probe microscopy has become an essential tool for studying on-surface reactions and molecular structures.

My presentation focuses on high-resolution scanning probe microscopy experiments combined with density functional theory to demonstrate recent highlights on the assembly of surface-supported low-dimensional carbon structures. In particular, the assembly and electronic structure of planar π -extended cycloparaphenylene macrocycles, which represent the first nanographene with an all-armchair edge topology, will be discussed [1]. [n]cycloparaphenylenes ([n]CPPs) have attracted significant attention due to their unique cyclic structure and highly effective para-conjugation leading to a myriad of fascinating (opto-)electronic properties. However, their strained topology prevents the π -extension of CPPs from converting them into armchair nanobelts or planarized CPP macrocycles. We have successfully tackled this long-standing challenge and present the bottom-up synthesis and characterization of atomically precise in-plane π -extended [12]CPP on Au(111).



Figure 1. Planar π-extended cycloparaphenylene synthesized by on-surface synthesis and characterized by scanning probe microscopy techniques.[1]

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Women's participation in inventive activity

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Myriads of brilliant women innovators contribute to solving some of humanity's biggest challenges.

The good news for Europe is that women's contribution to science and technology has increased in the last decades. Indeed, the women inventor rate, which measures the percentage of female inventors among all inventors in patent applications in a given year, has been increasing in Europe since the late 1970s.

This is one of the main findings of the study on "Women's participation in inventive activity" [1], conducted by the European Patent Office (EPO) based on its cutting-edge patent data. The study gives a picture of women and patenting as it stands today, providing evidence on the presence of women inventors across different countries, time periods and technology fields indicated in European patent applications received by the EPO.

On the other hand, the study shows that women remain persistently and disproportionately underrepresented among inventors in Europe.

The European figures are comparable to the US and slightly above Japan. But the gap is wider in Europe than in other parts of the world, especially in some Asian countries where high shares of women inventors constitute a major force for innovation.

The study reveals a pattern of a steadily decreasing share of women in the course of a STEM career - from PhD enrolment to PhD graduates in STEM (Science, technology, engineering and mathematics) to R&D personnel and researchers, to patenting. The pattern is broadly consistent across all European countries and confirms that women in Europe face increasing obstacles when progressing in STEM careers.

Increasing women's participation in science is a major challenge for Europe to address, as well as a key factor in its future sustainability and competitiveness.

There are positive findings from the study to build on and measures that can be taken, such as supporting the mobility of women scientists and promoting collaboration in research which may give women more opportunities to engage in careers related to inventions

It is also worth noting that patent applications from universities and Public Research Organizations have a significantly larger share of women inventors.

We need to ensure all voices are heard within our innovation ecosystem. From women to SMEs. From classrooms to careers.

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From surfaces physics to two-dimensional materials – and why you should not be afraid of serendipity

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The interaction of ion beams with surfaces and solids has been studied for decades. Famous physicists such as Bohr, Bethe, and Bloch have worked in this field, trying to describe the plethora of mechanisms that occur when an ion interacts with a solid. Nowadays, ion beams are well-established and reliable tools used, for example, in cancer therapy, in the semiconductor industry for doping, shaping and cutting, or for material analysis. On the other-hand, despite those early efforts, understanding of the fundamental mechanism at the microscopic level has not progressed very far because of the time and energy scales involved. Being a surface scientist by education, I have introduced two-dimensional materials as target material for the study of ion-solidinteractions. Due to their well-defined thickness, flexible preparation, and the wide range of available materials, they represent an ideal target material, and we have studied the interaction of ions of different types with surfaces [1] and 2D materials (see Fig.1) [2]. In my talk I will discuss different aspects of ions beams interacting with surfaces. I will relate these to the various stages of my own academic career in an attempt to show how the interplay of creativity, perseverance and, last but not least, serendipity has accompanied my scientific journey.



Figure 1. Folding of graphene and other 2D materials by ion irradiation. The sketch visualizes the backfolded graphene after an ion has impinged onto the surface under a grazing angle of incidence Θ (a) Foldings imaged by AFM in (1) single and bilayer graphene, (2) hBN, and (3) MoS₂. (b) The shape of the graphene folding pattern depends strongly on Θ . At larger angles, the pattern consists of multiple foldings oriented along low-indexed crystallographic directions of graphene as shown in the inset in (b), while under very grazing incidence the azimuthal angle determines the direction of the two foldings, which are aligned along the ion trajectory. The substrate also influences shape and size of the foldings. AFM images of suspended graphene show slits (c1), which are small foldings, as can be seen in atomically resolved TEM images (c2).

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A journey across the world for nano(carbon)materials

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In this talk, I would like to share my ongoing journey to learn about nano(carbon)materials and their application development. I will attempt to map changes in different aspects of my journey i.e., scientific training, career progression and geographic locations with changes in the nanocarbon world itself, through the eras of Fullerenes, Carbon Nanotubes (CNTs) and Graphene. My journey began with my fascination for Fullerenes as an undergraduate chemistry student in India through lectures and books. This fascination provided impetus to learn more practically about the worlds of nanotechnology/carbons through graduate studies. My first stop in practical training was at Sheffield, United Kingdom (UK) as a Masters student to train in assembling, manipulating and characterizing molecular entities for lab-on-chip applications. At the next stop of my training through doctoral studies at Cambridge, UK - I had the opportunity to further scale-up the first-hand-experience of designing macroassemblies from nanometric entities for realworld applications. At Cambridge, I focused on assembling CNTs continuously into kilometer-long wires and macroscale sheets exhibiting electrical, thermal and mechanical performances rivalling polymers and metals with industrialization potential [selected publications, 1-3]. The possibility of mass-producing and commercializing new high-performance materials for actual products steered me toward more applied research environments. I joined the National Institute of Advanced Industrial Science and Technology (AIST), Japan - an institution dedicated to bridging academic and industrial research. At AIST thorough postdoctoral training and as Japan Society for the Promotion of Science (JSPS) fellow and Staff research scientist, I concentrated on material development of metalnanocarbon composites for high-conductivity applications [selected publications, 4-8]. Here, the challenge was to harmonize well-established metal industry with commercially upcoming nanocarbon materials. With the strengthening of my inclination for materials research in realworld products, I joined Power Conversion Technology Laboratory, Huawei Nuremberg Research in October-2021. I now focus on a variety of materials including nanocarbons (like CNTs and graphene) to improve performances of existing and upcoming power electronic devices (power modules, inverters, etc.) for energy/automotive applications.

My journey through the nanocarbon world in India, UK, Japan and Germany has molded me to work with team-mates from and live in societies of different cultures. During this process, I have had the chance to observe and understand viewpoints – mine and others' - emanating from cultural, social and situational habits/reactions. The key lesson for me from my journey so far is: constructive outcomes in any realm (academia/industry/anywhere else) are possible only when power is used mindfully and responsibly. And when concerted and conscious effort is made to identify, focus and build on common ground, with awareness of tradeoffs, despite differences with mutual respect and tolerance.

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Shooting for sustainability

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The harnessing of solar energy to perform complex chemistries sustainably and on a global scale has been mastered by nature over 3 billion years ago with the emergence of photosynthesis. The ability to wire photosynthetic machineries to electrodes for photoelectrochemistry is a relatively new approach for studying photosynthesis. Additionally, this new ability allows us to re-wire photosynthesis, creating novel pathways for performing solar-energy conversion that is more sustainable than current methods.^{1,2}

My talk will be divided into three parts. First, I will give an overview of efforts in my lab to steal energy and electrons from photosynthesis.³⁻⁵ Second, I will briefly describe how I have forged my own science career path. Lastly, I will talk about key lessons gained from my personal journey as I strive to develop more sustainable ways of leading research and for producing green energy. I will also provide important insights gained from my involvement with several international women's forums,^{6,7}

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Flash Talks



Alternating Substrate-Ligand Coordination Provides a Lower Energy C-O Bond Cleavage Pathway for Electrochemically Driven Catalytic CO₂ Reduction

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Often Brønsted or Lewis acidic metal ions are employed to facilitate C-O bond cleavage in electrocatalytic CO₂ reduction. The former usually lead to non-selectivity, while the latter usually form insoluble carbonates in anhydrous conditions. My talk will be based on a ruthenium-polypyridyl catalyst framework, selective for CO production at a low overpotential, without necessarily requiring an additional acid or base.¹ The catalytic pathway embodies a metallacyclic intermediate which promotes C-O bond cleavage with lower activation barrier than the acyclic intermediate (Figure 1). Density functional theory and Fourier transformed infra-red spectroscopy, substantiate the involvement of the metallacyclic intermediate, made possible by: (1) the *flexible denticity* of the polypyridyl ligands, and (2) a metal center that can function as a Lewis base as well as a Lewis acid, in different steps of a single catalytic cycle.



Figure 1. Energetics of two different catalytic pathways for C-O bond cleavage.

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Colloidal Synthesis of 2D-Pnictogens: Antimonene and Bismuthene

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Pnictogens (P, As, Sb, and Bi) are emerging as promising 2D materials due to their exceptional properties, including layer-dependent bandgap, chemical reactivity, and spin-orbit coupling. However, the utilization of top-down methods for isolating these materials yields unsatisfactory outcomes due to interlayer interactions, hindering large-scale production.[1] A new bottom-up approach involving solution phase synthesis has been reported, enabling the large-scale production of well-defined hexagonal few-layer antimonene (FLA). The synthetic parameters have been optimized for producing high-quality FLA hexagons, and their implementation in a scalable process under continuous-flow conditions is being explored for optoelectronic device fabrication.[2] The colloidal synthesis approach has also been used to develop a novel synthesis of anisotropic few-layer bismuthene hexagons with excellent electronic properties.[3] This contribution demonstrates the potential of colloidal synthesis for preparing high-quality 2D-Pnictogens for electronic-grade application.

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CuInS₂ nanocrystals for solar-driven oxidation of redox mediators

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Copper indium sulfide quantum dots (CIS-QDs) are ternary semiconducting nanocrystals which have been studied in the last decades as an alternative to cadmium or lead-based QDs. One of their greatest advantages is their tunability, which allows CIS-QDs to be employed in many different areas, ranging from photocatalysis to bioimaging^{1,2}.

Our research aims to employ CIS-QDs as anodic material in photoelectrochemical cells for the oxidation of redox mediators.

CIS-QDs were attached to the FTO-TiO₂ photoanodes and a shell of CdS was deposited to improve the performance. The functionalized electrodes (TiO₂@CIS@CdS) were tested in ascorbate, sodium sulfide and TEMPOL aqueous solution. In future studies, we would like to test TiO₂@CIS@CdS photoanodes with different molecules, to get a deeper understanding of the oxidizing power and interfacial properties of the deposited CIS-QDs.

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On the Rich Photophysical Properties of Nitrogen-Containing Molecular Nanographenes and their Coordination Compounds

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Molecular nanographenes represent a promising candidate for optoelectronics and energy applications, in view of their intriguing and tunable optical and electrochemical properties [1]. We report on the rich photophysical properties of two nitrogen-containing fully benzenoid nanographenes, that is, sP and NG, and their corresponding coordination compounds featuring ruthenium porphyrin (RuP), that is, sP-RuP and RuP-NG-RuP (Figure 1). The lateral extension of the aromatic core when going from sP to NG, and the consequent symmetry decrease, resulted in an intriguing modulation of the photophysical properties. For example, NG shows a fluorescence quantum yield close to unity and thermally activated dual fluorescence from both S_1 and S_2 . Regarding the coordinative compounds, in sP-RuP an ultrafast energy transfer from the singlet excited state of sP to RuP is observed. Instead, in RuP-NG-RuP a "ping-pong" energy transfer, namely from NG to RuP and back to NG, is reported.



R: tert-butyl; R': dodecyl

Figure 1. Structures of the studied compounds.

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A Phenolate-Carbene Supported High-Valent Fe–O Intermediate Derived From Dioxygen

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Soluble methane monooxygenases utilize dioxygen to transform methane into methanol by breaking the 105 kcal/mol C–H bond.^[1] Recently, porphyrin-like tetracarbene macrocycles broadened the scope of suitable ligands in the biomimetic chemistry of Fe-mediated O₂ activation.^[2] The dimeric iron(II) complex [Fe(OCO)(MeCN)]₂ (1), supported by the bisphenolate carbene (OCO) ligand, was synthesized and characterized by single-crystal X-ray diffraction analysis, spectroscopic methods, and magnetization measurements. In solution, at rt, 1 activates O₂ to yield the asymmetric, μ -oxo-bridged [(OCO)Fe(μ -O)Fe(O(C=O)O)] (2). In 2, one of the Fe–C bonds was oxidized by one of the dioxygen atoms, while the other bridges the two Fe units. At –80 °C, a purple intermediate 3 is observed. Spectroscopic studies indicate iron(III) sites with one phenoxyl radical on each ligand. The absence of O–O vibrations in the resonance Raman spectrum of 3 suggests a symmetric diamond core structure [{(OCO)Fe₂(μ -O)₂] in 3.



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Recent advances in the modification of surface characteristics and functionality of plant proteins

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Plant proteins have recently gained increased popularity due to their availability, nutritional composition, low cost and suitability for sustainable production. However, some modifications based on physical, chemical and biological approaches may be required to modify the surface characteristics and functionality of plant proteins before they are widely used as an alternative to animal counterparts [1]. Emulsifying and foaming properties of plant proteins are highly dependent on the surface hydrophobicity, presence of reactive groups on the protein surface, net surface charge, and surface activity [2]. Novel physical processing techniques including microwave, pulsed electric fields, ohmic heating, ultrasound, radiofrequency, ionizing radiation, ozone, cold plasma, high pressure, and UV-C have been shown to be promising techniques in altering the surface characteristics and improving the functionality of plant proteins [1,3].

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Ultrathin ALD coatings on complex geometries for sensing and catalytic applications

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Atomic layer deposition (ALD) utilizes self-limiting surface reactions to construct ultrathin films layer by layer. Among many deposition techniques, ALD uniquely offers conformal deposition and excellent coating thickness control. Hence, the technique is particularly attractive for depositing structures with complex geometries, such as spheres, foams, 1D nanostructures, and 3D-printed structures.^[1-4] This leads to improved electrical, mechanical, optical, and chemical properties or adding new functionalities to the host structures.^[5–11] The presentation will discuss some ALD inorganic and semiconductor coatings on various scaffolds, the influence of the surface properties, their advantages and limitations. We will demonstrate that thin films in nanometer thicknesses are optimized for sensing and catalytic applications.^[7–11]

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Effect of vitamin B₆ on the formation of non-enzymatic protein modifications in heat-treated whey

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Whey-based foods are thermally processed to achieve desired technological properties and microbial safety. This is accompanied by the heat-induced formation of non-enzymatic post-translational protein modifications (nePTMs), which can impair the biological value of the proteins [1]. By understanding how food ingredients affect the formation of nePTMs, reduction strategies can be developed.

Therefore, whey obtained from raw cow's milk was fortified with vitamin B₆ and heated simulating industrial conditions. After hydrolysis of the proteins, the resulting peptides were measured by microLC-ESI-MS/MS. For this purpose, a sMRM method was developed for the structure- and binding site-specific detection of nePTMs on the major whey protein β -lactoglobulin.

15 nePTMs were identified, localised at 42 binding sites and relatively quantified. Vitamin B_6 was shown to affect the formation of nePTMs in a structure- and site-specific manner. In conclusion, vitamin B_6 can inhibit nePTM formation. However, as opposite effects were also observed, it is important to further elucidate the physiological effects of nePTMs.

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Photocatalysis as a Tool to Tackle Global Warming

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The present global energy crisis and evident consequences of the climate change show urgency of accelerating investment in novel, environmentally clean, safe, and sustainable technologies. Photocatalysis presents eco-friendly and sustainable means for green fuels generation *via* solar-to-chemical energy conversion. A typical photocatalytic process starts with absorption of the light energy by a photocatalyst followed by the energy transfer to catalytic active sites at which chemical reactions occur. For example, the photocatalytic water splitting into the molecular hydrogen and oxygen enables the storage of the solar energy directly in the chemical bonds. The conversion efficiency of the photocatalytic process is critically dependent on the nanomaterials that mediate the light-initiated redox reactions. Exploiting novel semiconductors is required to further develop large-scale technologies. Herein, composite materials bring special synergetic properties such as high solar light harvesting ability by concomitant sufficient thermodynamic driving force to promote redox reactions. In this symposium, I will provide an overview of our studies utilizing composites based on covalent organic frameworks for photocatalytic water splitting and CO₂ reduction.



Characterization of Complex Colloidal Nanomaterials by Analytical Ultracentrifugation (AUC)

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AUC is a powerful tool to determine particle size, shape, composition and optical properties of organic, inorganic as well as hybrid colloidal systems. In our contribution, we will give an overview of AUC studies on different colloidal nanomaterials and their specific properties. We will show how AUC is used to study the colloidal stability of cetyltrimethylammonium bromide functionalized superparamagnetic iron oxide nanoparticles. Furthermore, AUC coupled with extinction detection is used to study the mass-dependent sedimentation coefficient distribution of InP quantum dots (QDs) while coupled with emission detection^[2] it is used to study the size-dependent emission spectra of CdSe/CdS QDs^[3]. Also, by AUC the disaggregation of carbon nano onion (CNO) clusters is investigated.^[4]

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Water-soluble gold nanoparticles stabilized by N-heterocyclic carbenes for applications in catalysis and medicine

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In recent years, N-heterocyclic carbenes (NHCs) have emerged as an alternative to thiol ligands for stabilization of gold nanoparticles (AuNPs) due to the formation of strong Au-C interactions and the facile derivatization of the NHC scaffold at the NP surface, which can be useful to implement the applications of AuNPs in biomedicine and catalysis.¹

In this work, two water-soluble mono- or bidentate NHC stabilized AuNPs (NHC@AuNPs) were formed from their corresponding Au(I) NHC complexes *via* the 'bottom-up' approach.² The NPs were characterized by various spectroscopic and analytic methods. The NHC@AuNPs were then tested for their catalytic activity towards the reduction of nitrophenol substrates as a model reaction. The more stable NHC@AuNPs were also tested for their application in photothermal therapy (PTT).²

More recent work involves functionalization of these NHC@AuNPs with carboxylic acid groups for future bioconjugation to peptides for targeted PTT treatment or fluorophores for intracellular tracking.

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Posters



Metabolomics as a tool for identifying lung response after exposing to ultrafine particles aerosols

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There is still not much evidence on effects of ultrafine particles (UFP) on humans. Metabolites are key regulators of cell phenotype and behavior. Therefore, the identification of regulated metabolites as a consequence of exposure may provide clues to underlying mechanisms. In order to study the possible effects of UFP on lung, a triple cell culture lung model was developed and exposed to different aerosols generated in the lab. Applied aerosols consisted of UFP with either high or low content of semi-volatile organic compounds (SVOC). After exposure to both SVOCs, cell lysates were measured with GC-MS using an untargeted metabolomic approach. Statistical analysis revealed that top features differentiating the effects of exposure to high content SVOC from clean air control were iminodiacetic acid and tryptophan, whereas for low SVOC, 5'-methylthioadenosine and 5-methoxyindoleacetate. Consistently, pathway analysis showed that purine metabolism was the top significant pathway in both SVOC groups. Moreover, tryptophan metabolism, which modulates immunity and inflammation, was enriched in both groups.



Vitamins as inhibitors against the formation of non-enzymatic protein modifications (nePTMs) in infant formula

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Whey-based infant formulae (IF) are designed to mirror the composition of human breast milk, providing proteins, lactose, vitamins and more. To ensure microbiological safety and extended shelf-life, IF are thermally processed, which subjects the proteins to various modifications. This may compromise the quality of the proteins, especially considering essential amino acids for which IF are the only source for neonates [1].

To screen for potential inhibitors of nePTM formation, 14 vitamins were tested for their ability to protect β -lactoglobulin against oxidation, primary and secondary Maillard-, deamidation and transamination reactions. Therefore, raw whey was fortified with vitamins and heated simulating industrial conditions. After protein hydrolysation, the resulting peptides were measured by microLC-ESI-MS/MS (sMRM mode).

Vitamin B₁₂, one of the most promising inhibitors tested, was able to attenuate the formation of almost all 15 nePTMs monitored. Particularly notable is the decrease of modifications to the essential lysine resulting in lactulosyllysine as a primary and N^{ϵ}-carboxymethyllysine and N^{ϵ}-formyllysine as secondary Maillard-reaction products.

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Windmill-HBCs: Synthesis and Characterization of Novel Threefold Substituted HBC-Derivatives

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The investigation of graphene related compounds with non-zero band gaps, such as Hexa-*peri*-hexabenzocoronene (HBC), became of major interest in recent years.^[1] The opto-electronic properties of these molecules can be influenced easily by π -extension. ^[1, 2] Especially threefold substitution of HBCs indicates interesting changes in the absorption behavior, but only a few examples are reported. ^[2, 3] Here, we present a new strategy for the synthesis of a threefold iodinated HBC derivative. This molecule can serve as ideal precursor to generate C₃-symmetrical compounds and can undergo further cross-coupling reactions. First, different heteroatom-free substituents were connected to the HBC moiety via acetylene spacers to extend the π -system. Furthermore, N-containing substituents were coupled to the HBC. These molecules could serve as promising ligands for metal complexes. The influence on the optoelectronic properties of the presented HBCs were analyzed by UV/Vis and fluorescence spectroscopy.

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[C₂C₁Im][OTf] on Au(111) in UHV: A combined STM, IRAS, DFT and MD study

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In a solid catalyst with ionic liquid layer (SCILL), ionic liquid (IL) coatings are used to modify noble metal catalysts to improve their selectivity. In order to understand the origins of this type of selectivity control, we performed model studies by surface science methods in ultrahigh studied the IL 1-ethyl-3-methyl-imidazolium vacuum (UHV). In specific, we trifluoromethanesulfonate [C₂C₁Im][OTf] on a Au(111) single crystal surface. We investigated the growth and thermal stability of ultrathin IL films by infrared reflection absorption spectroscopy (IRAS) in time-resolved and temperature-programmed experiments. We combined these spectroscopy experiments with scanning tunneling microscopy (STM) to obtain information on the orientation of the ions, the interactions with the surface, the intermolecular interactions, and the structure formation. In addition, we performed density functional theory (DFT) calculations and molecular dynamics (MD) simulations to support the interpretation of the experimental data.



The golden path to anticancer chemotherapy: highly cytotoxic cyclometallated gold(III)-dithiocarbamate complexes

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In the 1980s, auranofin, a gold(I) complex, was FDA-approved for the treatment of rheumatism diseases, and showed antiproliferative activities in cancer cells; which sparked interest into researching gold(I)/(III) compounds in chemotherapy.^[1] Gold(III) coordination compounds have shown promising cytotoxic effects *in vitro* and *in vivo*; however, their limited stability in physiological environment has been a challenge in drug discovery.^[2] Therefore, organogold complexes were investigated to provide the required stability under physiological conditions. Here, five novel organogold(III)-dithiocarbamate complexes featuring cyclometallated C^N ligands were synthesized and showed high antiproliferative activity against human breast cancer cells. Compound **C3** displayed cytotoxicity against MDA-MB-231 cells in the nanomolar range with moderate selectivity. Reactivity of **C3** towards a model thiol, N-acetyl-L-cysteine, *via* NMR, inferred a mechanism of action due to binding of cysteine to the Au(III). Thus, Cys-containing proteins that play a role in cancer mechanism, such as thioredoxin-reductases, should be further investigated.

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In situ spectroscopic and analytical techniques to monitor particle formation

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Understanding the formation mechanism of particles is fundamental for the rational design of functional materials. During particle formation, several closely entangled chemicalphysical phenomena occur over a broad range of sizes and time-scales.

In this contribution, the use of multiple and simultaneous *in situ* analytical and spectroscopic techniques to monitor the evolution of the reaction mixtures in real time will be outlined for various materials.^{1,2,3,4,5}

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Towards Patterned Functionalization of Graphene and Black Phosphorus Heterostructures

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Covalent functionalization has become a powerful tool for the modification of various 2D materials. Among these, black phosphorus (BP) as a novel, layered material shows very promising electronic properties, however, the biggest obstacle to overcome is its intrinsic instability.^[1] The formation of BP-graphene, van-der-Waals-based heterostructures prolongs the lifetime of BP^[2] and offers the potential for broad range, tailor-made modifications *via* covalent functionalization of the graphene layer.^[3] Hence, we present the successful formation and covalent functionalization in well-defined areas of a BP-G heterostructure, as well as of perylene diimide-mediated BP-G hybrids.

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Energy Release in a Molecular Solar Thermal (MOST) System using a Switchable Hybrid Catalyst

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Molecular solar thermal (MOST) systems combine solar energy conversion, storage, and release using switchable photoisomers.¹ One challenge is to control the energy release in an efficient and selective manner.² In our study, we investigated the energy release from the MOST system mPENBD/mPEQC by the porphyrin [5-(*p*-Carboxyphenyl)-10,15,20-tri(*p*-tert-butylphenyl)porphyrinato] cobalt(II) anchored to $Co_3O_4(111)$ (Figure 1). We prepared the hybrid catalyst by depositing a monolayer of the porphyrin on $Co_3O_4(111)$. We demonstrate that the catalyst shows high activity for catalyzing the energy release from mPEQC to mPENBD in liquid phase. By applying a potential of < -1.4 V_{fc}, we are able to reduce the catalytically active Co(II) center to Co(I) which leads to a much lower catalytic activity. The original activity is regained when the Co center is reoxidized. To test the stability of the system, we performed 85 conversion cycles. We do not observe deactivation or the formation of side products.



Figure 1. Schematic representation of the investigated system.

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Stability and Charge Localization of [1:1] and [2:1] Complex lons of [n]CPPs and (Li⁺@)C₆₀/C₇₀

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[n]Cycloparaphenylenes ([n]CPPs) are strained macrocycles, comprising only sp²-hybridized carbon atoms. In recent years. [n]CPPs have become of great research interest in the field of supramolecular chemistry since their special structure enables the formation of novel host-guest complexes. In this work, we investigate the gas-phase chemistry of noncovalent complexes of [n]CPPs with C₆₀, C₇₀ and the endohedral Li⁺@C₆₀. The [1:1] complexes, [10]CPP \supset C₆₀ and [10]CPP \supset C₇₀, are observed as radical cations and anions, while [10]CPP \supset Li⁺@C₆₀ is only observed as cationic species. Their stability and charge distribution are studied using energy-resolved collision-induced dissociation (ER-CID).

Considering the complexes with C_{60} and C_{70} , the ER-CID measurements reveal that complexes with the C_{70} core exhibit a greater stability and that the radical cations are more stable than the respective radical anions. [2:1] complexes of the ([10]CPP₂ \supset C_{60/70})^{+,/-+} type are observed for the first time as isolated solitary gas-phase species. Here, C_{60} -based [2:1] complexes are less stable than the respective C₇₀ analogues.

Regarding complexes with Li⁺@C₆₀, our experiments reveal a significant increase in stability for complexes featuring [n]CPPs.



Analysis of the peptide profile of pasteurized milk during storage

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Untargeted peptide profile analysis reflects various characteristics of milk that can be used for product optimization, quality assessment, or authenticity control [1].

In this study, changes in the peptide profile of pasteurized milk were investigated by performing two independent storage experiments, followed by untargeted analysis with a microLC-ESI-timsTOF Pro-MS/MS system, bioinformatics, and an evaluation by conventional and multivariate statistics.

As a result, seven peptides were identified that reliably and accurately reflect the storage of pasteurized milk, for three of which the correlation with storage time has already been described in UHT milk [2]. Furthermore, it could be shown that especially the number of peptides released from β -casein correlates with the duration of storage and that various proteases may be involved in releasing the peptides.

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Photogearing – A Concept for Translation of Precise Motions at the Nanoscale

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Molecular gearing systems allow the integration of multiple motions in a correlated fashion, to translate motions from one locality to another and to change their speed and direction. However, currently no powerful concepts exist to implement active driving of gearing motions at the molecular scale. Herein, we present a light-fueled molecular gearing system based on the hemithioindigo chromophore and evidence its superiority over passive thermally activated gearing. Translation of a 180° rotation into a 120° rotation is achieved while at the same time the direction of the rotation axis is shifted by 120°. Within such photogearing process, precise motions at the nanoscale can be shifted in direction and decelerated similar to macroscopic bevel-gear operations in an energy consuming way – a necessary prerequisite to employ gearing as an active component in future integrated nanomachinery.

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Noncovalent Binding Between Fullerenes and Protonated Porphyrin-tweezers in the Gas Phase Studied by ESI-MS

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The complex formation and stability of three tetrabenzoporphyrin-tweezers (TBP) with up to four fullerene guests was investigated by electrospray ionization mass spectrometry. The doubly protonated TBP-tweezers readily form complexes with C_{60} . Energy-dependent collision-induced dissociation experiments show successive losses of the neutral fullerenes, indicating noncovalent binding.

There are two likely complex geometries: A *"tweezer-like"* complex were one fullerene is enclosed from both TBP moieties while the other fullerenes bind to the outside of the TBP-tweezer, or an *"open"* geometry in which the fullerenes bind above and below the TBP units. Experimental results indicate that all [1:1] complexes adopt the "tweezer-like" geometry, while the structure cannot be determined experimentally for the [1:2] and [1:3] complexes. However, for the [1:4] complex, the structure opens up to provide a fourth porphyrin binding site for the fullerenes. In general, the [1:1] complexes are more stable than the larger complexes, the stability decreases with increasing number of fullerenes. This study shows that ESI-MS is a powerful tool for the study of noncovalently bound supramolecular complexes.



Heterogeneous water oxidation catalysis in porous materials

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Mimicking the oxygen evolving Photosystem II has been a successful strategy for the design of supramolecular architectures for homogenous water oxidation catalysis.^[1,2] The implementation of well-defined molecular water oxidation catalysts into crystalline framework materials would lead to heterogeneous catalysts with improved stability, recyclability and structural integrity. As one of the very few examples available in the literature so far, we recently reported on Ru(bda)-containing COF nanoparticles with excellent performance in heterogeneous water oxidation.^[3] Here, we expand on this concept and report on the incooperation of Ru(bda) units as linear building blocks in MOFs or the encapsulation of molecular WOCs in crystalline organic cages..

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NEW NORBORNADIENE-BASED DERIVATIVES AS PROMISING CANDIDATES FOR MOLECULAR SOLAR THERMAL TECHNOLOGIES

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One of the most promising approaches towards chemical energy storage is the utilization of so-called molecular solar thermal (MOST) systems. A very efficient MOST system is the norbornadiene/quadricyclane (NBD/QC) interconversion couple.^[1] By precise structural modifications of the parent carbon scaffold, a change of the related photophysical properties can be achieved. Thus, tailored NBD derivatives can be implemented and investigated regarding actual energy storage applications.^[2] Through variable catalytic stimuli, the back-isomerization from the high-energy QC to the parent energy-lean NBD is initiated on demand, resulting in the release of the stored energy.^[3] The presented library of functionalized NBD derivatives was tested regarding their photophysical properties as well as interconversion capability using ¹H-NMR and UV/Vis spectroscopy as main characterization methods. Hereby, electrochemical activation was investigated as a promising back-conversion stimulus.

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Synthesis of sugar-bridged fullerene dumbbells and pseudorotaxane formation with the [10]cycloparaphenylene nanoring

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We describe the synthesis and characterization of four dumbbell-shaped fullerene molecules bridged by isosorbide\isomannide moieties.* Their electrochemical behaviour and complexation with [10]cycloparaphenylene ([10]CPP) were also investigated. Cyclic voltammetry (CV) of fullerene dumbbells showed high electron affinity, highlighting their ability to interact well with electron-donating counterparts such as carbon nanorings, which are charge and shape complementary. Thermodynamic and kinetic parameters of complexation were studied by isothermal titration calorimetry (ITC) and additional information about binding stoichiometries was obtained by NMR titration experiments. Two different approaches were used, resulting in bridged cyclopropane- and furan-based structures. Regardless of the type of linker, all derivatives formed conventional 2:1 complexes [10]CPP₂ \supset C_{60derivative}. However, the methano-dumbbell molecules showed different binding behaviour as mono-, bispseudorotaxanes as well as oligomers (polymers) were detected. The formation of linear polymers could be of great importance for solar energy conversion processes.¹

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S- and N-substituted Hexa-peri-hexabenzocoronenes

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Even though the carbon-fluorine bond shows remarkable strength, the bond can be utilized to implement different functional groups into the molecule. In a nucleophilic fashion e.g., thiolates or nitrogen nucleophiles can substitute the fluorine, resulting in the corresponding S- and N-substituted derivatives.^[1-2] We report the synthesis toward a series of new mono-, di-, tri-, tetra-, and hexafluorinated Hexa-*peri*-hexabenzocoronenes (HBCs) and their reaction to the corresponding substituted derivatives, utilizing the substitution of fluorine. The electronic properties of these compounds were studied regarding the influence of the attached substituents and the substitution pattern. Moreover, the thioether-HBCs are of particular interest due to their versatile behavior towards oxidants^[3], or alkylation agents^[4] and were exemplarily transformed into the corresponding sulfones and sulfonium salts.

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Towards 2D Covalent Pattering of Graphene

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Covalent functionalization of graphene has become an important field of research, as it offers a precise modification of its intrinsic properties. By binding desired functional moieties in a spatially-resolved manner, regions with different chemical and physical attributes can be combined.^[1] Herein, we present a new approach towards mixed patterns using different halogenated dibenzoyl peroxides as model compounds,^[2] furthermore we present the patterned functionalization with a brand-new compound class, the perfluorinated phenyl azides (PFPAs), *via* laser- or electron-beam writing. Subsequent post-functionalization of the PFPA-functionalized graphene presents the first step towards a highly versatile material modification.^[3]

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Multiply-Fused Porphyrin Nanographene Conjugates

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The application of porphyrins as a main element for the design of extended carbon-based frameworks gained increasing popularity in recent years.^[1] The fusion of aromatic hydrocarbons of various sizes to the β - and *meso*- positions of porphyrins emerged hereby as a particularly convenient strategy for an effective expansion of the aromatic network.^[2] The extension of the π -system leads to substantial alterations in optical and electrochemical features. These changes involve a bathochromic shift in the absorption spectrum, increased absorption in the NIR range as well as a profound decrease of the HOMO-LUMO gap.

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Experimental Determination of Bond Dissociation Energies of Silver(I)-Helicene Adducts in the Gas-Phase by ESI-MS/MS

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[n]Helicenes (n = 6 and 7) are known to form [1:1] complexes with silver cations, where the helicene acts as a molecular tweezer, attaching to Ag^+ in a bidentate fashion. Our MS/MS experiments confirm the charge transfer from the Ag^+ to the [n]helicene during collision-induced dissociation (CID). We could experimentally determine the bond dissociation energy of the [8]helicene/Ag⁺ complex by calibration of the energy scale with the calculated energy values of Ag^+ complexes with [6] and [7]helicene. Besides the well-established [1:1] helicene/Ag⁺-complex in which the helicene provides a tweezer-like surrounding for the Ag⁺, there is also a [2:1] complex formed. Density-functional theory (DFT) in conjunction with energy-resolved collision-induced dissociation (ER-CID) experiments reveal that the second helicene attaches via π π -stacking to the first helicene which is part of the pre-formed [1:1] tweezer complex with Ag⁺. For polycyclic aromatic hydrocarbons (PAHs) of planar structure, the [2:1] complex with silver(I) is typically structured as a Ag⁺-bound dimer in which the Ag⁺ would bind to both PAHs as the central metal ion (PAH---Ag⁺---PAH).



Carbon Nanocages for Supramolecular Interactions

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Carbon cages as nanoarchitectures possessing hollow interiors are of great interest in fundamental supramolecular chemistry (endohedral guest binding) and might also find applications such as catalyst, selective recognition, sensoring and drug delivery systems. We target the synthesis of carbon-rich void hosts such as cyclophanes and tweezers for selective carbon allotrope recognition and other supramolecular interactions such as chiral self-sorting. Our work comprises representative prototypes of PAH cages based on functional dyes such as perylene bisimides (PBIs)¹ as well as curved buckybowls building blocks.² Their application in the formation of diastereoselective products,^{3,4} tunable cavity for host-guest encapsulation, pseudorotaxane formation⁵ and selective fullerene binding demonstrate their huge versatility.

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In situ Atomic Force Microscopy (AFM) of (electro)catalytically active interfaces

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Atomic Force Microscopy (AFM) is a highly sensitive method to morphologically characterize interfaces independent from the support properties (e.g. electrical conductivity). With our new in situ AFM setup (including a Cypher AFM device; Oxford Instruments), we are able to study various surfaces under in situ conditions e.g. gas/solid, liquid/solid, and electrochemical interfaces. We are able to precisely control the experimental parameters such as temperature, pressure, the composition and flow rates of gases and liquids, and the applied potential. Overall, this allows us to study (electro)catalytically active interfaces and (solution) atomic layer deposition processes under (or close to) reaction conditions. Specifically, we will investigate in a first step the influence of ionic liquids on the corrosion of electrode materials such as Au(111).

The setup is capable of fast scanning and we achieve highest (down to atomic) resolution even under such extreme conditions. The availability of a laser-driven thermal excitation ensures stable and constant amplitudes of the cantilever while scanning in tapping mode, even in highly viscous environments such as ionic liquids.



Enzyme mapping to elucidate the role of endogenous proteolytic enzymes on the native peptide profile of bovine milk

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Cow's milk usually contains about 3.5 % (w/w) total protein, the main fraction being caseins [1]. Milk also contains proteolytic enzymes which recognise certain amino acids in milk proteins as cleavage sites, thus, they contribute to the native milk peptide fraction [2]. To gain more insights into the cleavage behaviour and specific cleavage sites, the most common milk enzymes were separately incubated with a casein solution. Peptides were analysed using high-resolution mass spectrometry and bioinformatic techniques. Results showed that e.g., cathepsin D and plasmin have high specificity, while e.g., elastase cleaves after uncharged, non-aromatic amino acids in general. Furthermore, a cleavage pattern was created for each individual enzyme. A principal component analysis showed that the cleavage pattern and the enzyme activity depend on the enzyme species. The results from the model were confirmed by analysing the native peptide profile of raw milk.

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Optical Properties of Hexa-*peri*-hexabenzocoronenes and Perylenes in Hybrid Systems

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Hexabenzocoronene- (HBC) and perylene derivatives were synthesized as well-designed building blocks of nanographene hybrid compounds. These are aimed at applications in organic photovoltaics and optoelectronics due to precise combination and tuning of their properties.

The study focused on examining the influence of π -system modification, interaction with the environment (e.g. solvent effects) and combination of different moieties in non-conjugated HBC-benzimidazole and -perylene hybrids. The resulting properties were analyzed *via* UV/Vis- and fluorescence spectroscopy and cyclovoltammetry. Firstly, the colour of perylene monoimide-monoanhydride and π -extended perylene-benzimidazoles in solution is primarily affected by the molecules' ability for H-bonding rather than polarity of the solvents. A colour transformation from orange to purple was detected upon decreasing π -conjugation in an oxidized HBC-bisdiketone. Furthermore, the characteristic colours of the precursors (blue, yellow) were combined to green in a perylene-HBC hybrid compound.

This research emphasizes the versatility and property-controllability of these hybrid molecules, enabling accurate tailoring of materials for desired applications. Future challenges include π -extension through acetylene bridges and the introduction of other optically active building blocks.



Rylene Bisimide Cyclophanes with Versatile Cavities and Their Host-Guest Interactions

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Among different types of macrocycles, cyclophanes have reached special interest in the last years due to their rigid structures and aromatic moieties which enable a large variety of applications in supramolecular chemistry. A rather new class are the rylene bisimide cyclophanes. The open cavity is ideally suited for the encapsulation of guest molecules between the two π -surfaces, which can be studied by absorption and emission spectroscopy. Additionally, the rigidified structure allowed to study the dependence of the linker length on the interaction of the chromophores of empty PBI cyclophanes could be studied.^[1] In a new hetero-cyclophane a chirality- and energy transfer across the cavity could be observed.^[2] Recent results including newly synthesized cyclophanes will be presented, including their interaction with a large variety of guest molecules.

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Raman and photoluminescence studies on twisted bilayer CVD-grown MoS₂

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Twisting two monolayers of MoS₂ on top of each other gives a new tuning parameter to the system, namely the twist angle. Depending on the twist angle we observe characteristic optical features with Raman and photoluminescence spectroscopy such as the appearance of moiré phonon modes and energy shifts of the excitonic transitions. Chemical vapor deposition (CVD) was used to produce clearly separated, triangular shaped MoS₂ monolayers. Using such CVD-grown monolayers, twisted bilayers are manufactured with twist angles between 0° and 60°. Here the fabrication of such twisted bilayers and their optical features shall be presented.



Heterogeneous Electrochemical Water Oxidation Catalysis With Linear Ru(bda) Oligomers

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Ruthenium-based coordination oligomers are known as highly active and stable heterogeneous catalysts for electrochemical water oxidation on carbon nanotube support.^[1] We report the synthesis of a series of Ru(bda) (bda = 2,2'-bipyridine-6,6'-dicaboxylate) oligomers with varying length and linker size. Heterogeneous electrochemical water oxidation is achieved with high TOF (\sim 6×10³ s⁻¹) and record TON (\sim 2×10⁷) values.

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SYNTHESIS AND CHARACTERIZATION OF AMPHIPHILIC PORPHYRIN-PERYLENEBISIMIDE ARCHITECTURES

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An efficient way to address the challenge of tailoring the supramolecular assembly of donoracceptor (D-A) systems lies in the utilization of the hydrophobic effect by the synthesis of integrated amphiphiles, consisting of suitable D-A couples, which has already been showcased in exemplary systems.^[1,2] Architectures built from porphyrins and perylenebisimides (PBIs) are well-understood D-A systems and inherit remarkable properties,^[3] but still, to this day, amphiphilic derivatives based on these couples are only sparsely explored.^[4] Herein, we report the synthetic approach towards a family of highly watersoluble porphyrin-PBI bola-amphiphiles. This was achieved by the utilization of oligocarboxylic acid-capped Newkome dendrons. Synthetic modification of the PBI core`s geometry and dendron size gave first insights into the structure-to-function principles regarding aggregation behavior.

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Exploring the potential of CXCR4 mimetic peptides to target cancer cells

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The chemokine receptor CXCR4 is involved in many physiological processes, as well as in diseases, including HIV-1 infection and cancer.¹ CXCR4 interaction with the chemokine CXCL12 has been demonstrated to stimulate different cancer processes.² In HIV-1 infection, on the other hand, CXCR4 serves as a coreceptor for virus entry into the host cell.

The extracellular domain of CXCR4, i.e. the N-terminus and extracellular loops (ECLs), are important for receptor function and ligand binding.³ We are exploring the potential of CXCR4 mimetic peptides, derived from the extracellular domain, to interfere with the proliferation of CXCR4/CXCL12-dependent cancer cells.

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Insights into the Morphology and Size Distribution of Carbon Nano Onions: An In Depth Analysis

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Carbon Nano Onions (CNOs) are spherical nanoparticles of varying sizes composed of concentrical multi-layered fullerenes, discovered in 1992.^[1] The CNOs graphitic multilayer structure and outstanding properties, such as low density, large surface area and high thermal stability make them promising candidates for a variety of applications. Particle size and agglomeration behaviour of CNOs varies significantly depending on the preparation method, which include: pyrolysis, arc discharge and thermal annealing of nano diamonds. The thermal annealing method in particular, while flexible in regards to final CNO size and morphology, can produce large particle clusters, interconnected and encapsulated by graphitic shells.^[2] Purified and oxidized CNOs are obtained by applying an acidic work up, improving their properties by de-clustering the CNOs to even monodispersed particles. Utilizing analysis methods such as High Resolution Transmission Electron Microscopy (HRTEM), Dynamic light scattering (DLS), ζ -Potential Measurements and Analytical Ultracentrifugation (AUC), CNOs are characterized in depth.

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Impact of physicochemical parameters of human skin on 1,4dioxane and hydrofluoric acid absorption

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The aim of the study was to investigate the effect of intradermal pH (chemical) and skin temperature (physical) on the absorption of hydrofluoric acid (HF) and 1,4-dioxane. In diffusion cell experiments, transdermal uptake of fluoride (fluoride-sensitive electrode) and 1,4-dioxane (headspace GC-MS) was investigated over 8h. Intradermal pH was set to 7.2 or 6.5, and skin temperatures to 32°C or 24-25°C. At low pH, absorption increased for fluoride (1.7x) and remained unchanged for 1,4-dioxane. The maximal fluxes at low and high pH were 30 and 13.8µg/h/cm² for fluoride and ~40µg/h/cm² for 1,4-dioxane. The respective lag times of fluoride were 20 or 44 min and ~2 hours for 1,4-dioxane. At low temperatures, absorption decreased 1.3-fold for fluoride and increased 1.8-fold for 1,4-dioxane. Flux values were high for fluoride at 32°C and for 1,4-dioxane at 24°C. Thereby lag time was halved for fluoride and decreased by 25% for 1,4-dioxane. The amount and kinetics of absorption of both substances showed to be temperature- and pH-dependent, emphasizing the impact of physicochemical variations on absorption.



Shell-by-Shell Functionalized Nanoparticles as Supramolecular Mediator in the Photosensitized Conversion of Norbornadiene to Quadricyclane in Aqueous Media

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In 2015 our group has established a novel universal wet-chemical two-step Shell-by-Shell-(SbS)-functionalization-approach of metal oxide nanoparticles (NP) with phosphonic acids in the 1stshell and tailor-made amphiphiles in the 2ndshell.^[1] Work based on this concept has shown that driven by hydrophobic interactions the incorporation of apolar molecules in the SbS-architecture is possible.^[2] Combining this approach with the molecular solar thermal (MOST) energy storage system norbornadiene (NBD)/ quadricyclane (QC)^[3] enables the conversion of NBD into its metastable and energy-rich isomer QC in aqueous media. Within this work it is shown that providing hydrophobic NBD and photosensitizing agents to an aqueous dispersion of SbS-functionalized NPs makes it possible to incorporate huge amounts of MOST-molecules. By exposing to light the conversion to QC inside these SbS-systems can be observed. For analysis and quantification DLS, ζ -potential, and GC/MS techniques are used.

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Mass Spectrometry Study of Host-Guest Complexes between Angle-Strained Alkyne-Containing Cycloparaphenylenes and Fullerenes

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Cycloparaphenylenes (CPPs) are strained ring molecules, comprising only sp² hybridized carbon atoms. In this study, a variety of functionalized triazole-containing CPPs with an elliptic lasso-like shape are exploited as hosts for C₆₀ and C₇₀. Host-guest complexes of these Lasso-CPPs with C₆₀/C₇₀ are investigated by electrospray ionization mass spectrometry. The mass spectra show that [1:1] and [2:1] complexes of Lasso-CPPs with C₆₀/C₇₀ are formed as radical cations and protonated species. Energy-resolved collision (MS²) experiments reveal that Lasso CPP⊃fullerene [1:1] complexes are more stable as radical cations than as protonated species. Changes in the electron donating/accepting nature of substituents on Lasso-CPPs, however, have little influence on the complex stability. Additionally, MS² experiments indicate that complexes of Lasso CPPs with C₇₀ are more stable than the corresponding C₆₀ analogues ^[1].

Our results suggest that strain-promoted Lasso-CPPs are desirable host molecules for fullerenes. Mass spectrometry is a powerful tool for the study of these non-covalent host-guest complexes.

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Tuning the morphology of spray-dried supraparticles: effects of building block size and concentration

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Supraparticles, assemblies of nano building blocks, are widely applied in chemical, pharmaceutical, and food industries. ^[1] The resulting properties of supraparticles can be controlled via not only the properties of the nanoparticle building blocks, but also the supraparticular morphologies. ^[2] In this study, nanoparticle sizes, concentrations, and weight ratios were varied to obtain different structures of supraparticles via spray-drying. It is found that small nanoparticles form a flexible shell during the spray-dry process, resulting in mushroom cap-like supraparticles, while larger nanoparticles tend to form spherical supraparticles. When small nanoparticles outweigh large ones in binary or trinary dispersions, smooth and non-spherical supraparticles can be produced. Thus, supraparticles of hierarchical structures can be controllably achieved via spray-drying multimodal-sized building blocks, which can be useful for diverse applications e.g. catalysts, energy storage devices, or markers.





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Women in Science 2nd Erlangen Symposium June 18-20, 2023 Erlangen, Germany

Our main goal is to tackle the underrepresentation of women in science by increasing the visibility of female researchers and by fostering conversations among all genders on how we can achieve gender equality in science.



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