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26th JCF Spring Symposium

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I1

Rethinking Chemistry@ALTANA - How Specialty Chemicals Help Shaping a Greener Future

As a specialty chemical company, ALTANA develops high-quality and innovative chemical solutions. ALTANA's four divisions – BYK, ECKART, ELANTAS, and ACTEGA – have set worldwide standards in their markets. Our innovative products enable companies to develop future technologies today, technologies that make life easier, safer, and more comfortable.

Identifying, developing, and realizing solutions towards a greener future is a key component of ALTANA's corporate strategy. However, the global path towards a greener future is challenging and requires multifaceted efforts. ALTANA meets this challenge by rethinking internal processes and becoming climate neutral as soon as 2025. Due to ALTANA's market leadership in key future markets, ALTANA is in the position to leverage its sustainable solutions and serve as a sustainability enabler for entire industry branches.

I2

Insights and entry opportunities at BASF

Luna Wiesner

BASF
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What makes working at BASF special?

Our strength is the solidarity and close cooperation of our teams. We call it the power of connected minds!

By creating a safe and inspiring work environment and acting responsibly, we motivate our employees to achieve exceptional performance. This active commitment of our employees ensures our long-term success.

The best team is the key to our success.

Our employees make a significant contribution to BASF's success: We rely on the engagement of our employees and give them the tools and skills necessary to be able to offer our customers differentiated and customized products, services and solutions.

BASF is a great place to build a rewarding, successful career: We cultivate a working environment that inspires and connects people. It is founded on inclusive leadership based on mutual trust, respect and dedication to top performance.

Come create chemistry with us!

I3

Digitalization and AI in Drug Discovery

Boehringer Ingelheim

Everyone is talking about the transformative power of digitalization & AI, but how are digital technologies really being applied in industrial research? And how do they help scientists at Boehringer Ingelheim invent molecules that could become drugs one day?

In this talk from the medicinal chemist's perspective, you will get a glimpse of how scientists collaborate with machines by using a range of digital tools at Boehringer Ingelheim to generate ideas for the drugs of the future.

I4

Green Hydrogen: Europe’s Sustainable Future with ZSW’s Innovations

Markus Hölzle

Professor Markus Hölzle from ZSW will highlight hydrogen's crucial role in shaping Europe's sustainable energy future. With the EU's ambitious targets for hydrogen deployment by 2050, this presentation will explore the benefits of green hydrogen production and ZSW's contributions in advancing hydrogen technologies. Attendees will gain insights into how hydrogen can mitigate CO_2 emissions and drive socio-economic growth, as well as how ZSW facilitates technology transfer for companies to participate and profit from the sustainable hydrogen pathway.


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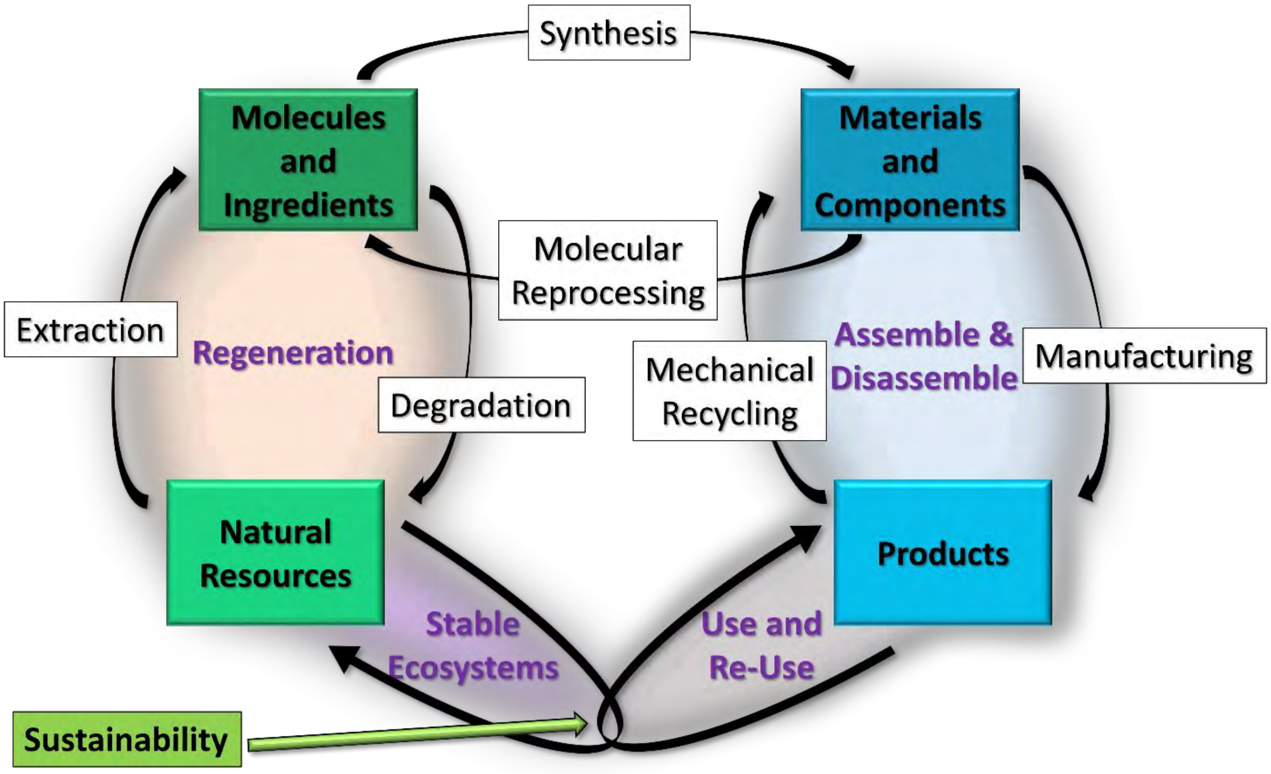
K1

The "Islands of Innovation": Green Chemistry from the bench to society.

John C. Warner [1,2]

[1] *Technology Greenhouse, LLC Woburn, MA, USA*
[2] *Monash University, School of Chemistry, Victoria, Australia*

Often people refer to bodies of chemistry as being "applied" or "fundamental". This presentation will discuss the problems that occur from these characterizations. While the mindset and bias of the individual carrying out the chemistry might be "applied" or "fundamental" the chemistry is neither. The author's metaphor of his "Islands of Innovation" will be presented to illustrate how concepts pass through intellectual territories of molecules, molecular mechanisms, materials mechanisms, materials properties and products. Several illustrative examples of green chemistry will be presented.



K2 Chemistry Europe Lecture

Hybrid Materials for Energy Conversion Toward Smart Photovoltaics

Jovana V. Milić
Jovana.milic@unifr.ch
Adolphe Merkle Institute, University of Fribourg, CH-1700 Fribourg, Switzerland

Hybrid organic-inorganic materials are increasingly relevant for emerging energy conversion technologies. In particular, metal halide perovskites have become one of the leading semiconductors for solar-to-electric energy conversion in photovoltaics.[1–2] However, their operational instability hinders practical applications. While this can, to an extent, be overcome by incorporating organic moieties within hybrid perovskite frameworks that form low-dimensional architectures with superior operational stabilities, their electronically insulating character often compromises the resulting performances.[2–3] This has been addressed by relying on the supramolecular engineering in the design of (photo)electroactive organic species that can enhance the functionality of hybrid perovskites by enabling their control in response voltage bias,[4] light,[5,6] and pressure,[7] opening a path toward multifunctional materials and smart photovoltaics.

Figure 1: Schematic representation of multifunctional hybrid materials.

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K3

Organic Solar Cells – From the Research Lab into the Classroom

Amitabh Banerji [1]

[1] *University of Potsdam, Chemistry Education, Germany*

To prepare students for a life in an increasingly technology dominated world and to motivate them for STEM (science, technology, engineering, mathematics) it is crucial to implement cutting-edge research and future technologies into the science curriculum of schools and universities. Our group has a long-lasting expertise in introducing recent scientific developments, i.e. semiconductors based on organic and perovskite materials into the curricula of German schools and universities, following the principles of Curriculum Innovation [1].

Organic semiconductors are a new class of materials representing an innovative field of scientific research. Efficient illuminants, such as organic light emitting diodes (OLEDs) can be found in ultra-thin and super-bright displays of modern high-tech applications. Organic Photovoltaic cells (OPV) can be produced as light weight, super-thin, flexible and semi-transparent films, which can be embedded into the windows and facades of modern buildings.

In my talk, I will discuss the theoretical basics of organic solar cells and I will demonstrate the low-cost fabrication of a DIY-OPV-cell [2] in a live demo (fig. 1). Furthermore, I will present our newest development: a low-cost fuell-cell made from a tic-tac-box [3] and I will try to produce green-hydrogen in a small-scale experiment.

Science can be so much fun!

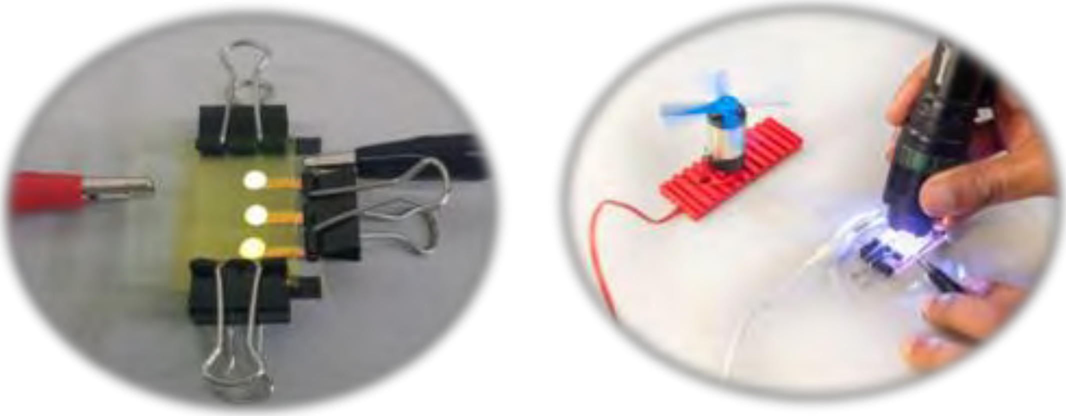

Figure 1: low-cost DIY-OLED (left) and DIY-OPV-cell (right)

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K4

The design of highly porous materials for globally relevant gas and liquid separations

Shuliang Yang, Daniel T. Sun, Li Peng, Vikram V. Karve, Natalia Gasilova, Mehrdad Asgari, Emad Oveisi, Olga Trukhina, and Wendy L. Queen

[1] *Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne (EPFL) Sion, Switzerland*

Among several classes of porous materials, metal-organic frameworks (MOFs) are particularly attractive due to their unprecedented internal surface areas (up to 7800 m^2/g),[1] easy chemical tunability, and strong, selective binding of a host of guest species. Through judicious selection of MOF building blocks, which include metal ions and organic ligands, one can readily modify their properties for a variety of potential applications. Despite these attractive features, there are still challenges in the field that limit our ability to use MOFs as a solution for a wide range of industrial problems. For instance, some MOFs have limited mechanical and chemical stability, particularly in highly humid, acidic or basic environments. Overcoming this problem could lead to extended lifetimes and hence increased feasibility for their use in areas where such conditions are required.

In response to these needs, we have recently begun to combine MOFs and polymers in an effort to boost MOF performance and extend their stability.[2] Our recent work demonstrates that selected polymers can significantly enhance MOF performance in a number of important liquid and gas separations[3-7] as well as extend catalyst lifetimes in selected reactions.[8-9] In addition to this, controlled polymerization processes were employed to enhance the mechanical stability[10] of large pore frameworks and extend the chemical stability of a number structurally diverse MOFs not only in humid environments, but also in acidic and basic media.[11] We hope such work can help bring these frameworks a few steps closer to their deployment into a range of ecologically and economically important applications. In this presentation, our recent work, devoted to the development of novel MOF polymer composites specifically for globally relevant separations, will be outlined.

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K5

Building Blocks obtained from Carbohydrates and Amino Acids using Electroorganic Synthesis and Photocatalysis

Sebastian B. Beil [1]

[1] *University of Groningen, Stratingh Institute for Chemistry, Groningen, The Netherlands*

Complex and three-dimensional organic molecules are modern entry points in drug discovery.[1] An increasing global demand for new therapeutics, based on natural or tailored substrates, is urging for the development of new chemistry. Nevertheless, their synthesis is more difficult since adequate fragments are elusive thus hampering new patient treatments in a timely manner. Utilizing small aliphatic natural building blocks facilitates a sustainable approach towards drug molecules with a high C(sp3) content. By applying single-electron disconnections to their synthetic design, large amounts of waste and timely reaction sequences can be circumvented to obtain new molecular targets. The mild activation modes obtained from electroorganic synthesis[2-3] and photocatalysis form transient radicals, which can undergo functionalization or cross-coupling reactions when merged with first-row transition metal catalysis, like nickel and copper.[4] Thus, endergonic chemical reactions, become feasible at ambient conditions.

In our group, we utilize photoredox catalysis as tools to access non-natural amino acids from their natural counterparts.[5-6] The photochemical conversion of amino acids through high-energy radicals will yield pharmaceutically relevant non-natural amino acids which offer vast opportunities to discover new building blocks for next-generation medication. In addition, we use carbohydrates and convert them into building blocks for materials applications by the use of electroorganic synthesis.[7-8] By combining natural building blocks as resources with electrosynthesis and photocatalysis we aim to improve existing strategies thus rendering more sustainable ones.

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A1 Dres. Volker and Elke Münch Prize for Science and Research 2023

Adsorption of chlorine: Polymers as efficient chlorine storage matrices at ambient conditions

Alejandro Lorente, Merlin Kleoff, Olaf Wagner, Rainer Haag, Sebastian Riedel

Institut für Chemie und Biochemie, Freie Universität Berlin, Berlin D-14195, Germany

Chlorine is one of the most important basic chemicals in the chemical industry. Approximately 50 percent of all industrial chemicals, 30 percent of all agricultural chemicals, and 20 percent of all pharmaceuticals require chlorine for production.[1] However, the production of chlorine is one of the most energy-intensive processes in the chemical industry. Additionally, chlorine is stored either by pressure liquefaction at 7 bar or by cooling below the boiling point of -34 °C.[2] Both methods are energy-intensive and require circumstantial corrosion protection and safety concepts in case of a failure of the storage system, leading to the release of toxic chlorine gas.

Recently, the adsorption of chlorine at ambient conditions was demonstrated through the use of quaternary ammonium salts.[3] Nevertheless, the resulting product is an ionic liquid after adsorption, which limits its application in some industrial processes. In our research, we have developed a new macroporous, three-dimensional crosslinked polymer cryogel with high surface area and increased thermal stability and other polymer composites. The adsorption of chlorine was achieved in its solid state, making it highly desirable for various industrial applications such as safer and more efficient storage and transportation, or the purification of residual gas streams.

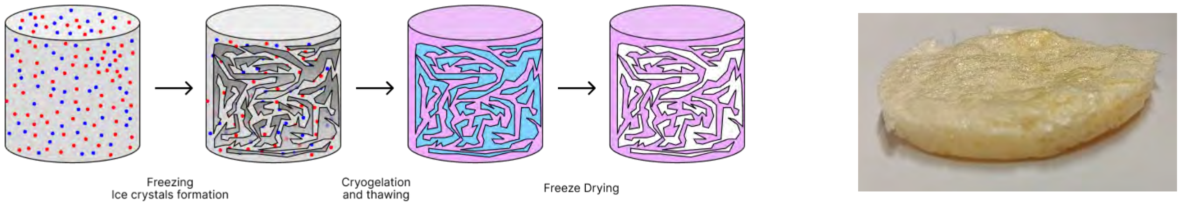

Figure 1. General diagram of the steps occurring during the cryogelation process (left). Physical appearance of the cryogels after final drying process (right).

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Enantioselective Electrochemical Cobalt-Catalyzed C–H Activation

Tristan von Münchow, Suman Dana, Ye Lin, Yang Xu, Binbin Yuan, and Lutz Ackermann*

Georg-August-Universität, Institut für Organische und Biomolekulare Chemie (IOBC) &
Wöhler Research Institute for Sustainable Chemistry (WISCh), Göttingen, Germany

In recent years, the merging of electrosynthesis with enantioselective C–H activation has evolved as a powerful and sustainable technique that enables the important hydrogen evolution reaction (HER) being paired to the synthesis of chiral valuable molecules.[1] This approach allows to perform oxidative transformations without the use of sacrificial stoichiometric oxidants. Further advantages in terms of sustainability and resource economy result from the use of catalysts based on earth-abundant transition metals instead of expensive 4d and 5d transition metals.[2] However, enantioselective electrochemical C–H activation through 3d transition metal catalysis represents a challenge and remained unexplored until very recently.

Herein, we describe strategies for enantioselective cobaltaelectro-catalyzed C–H activations that allow the synthesis of versatile chiral molecules.[3] Thus, the developed electrooxidative cobalt catalysis provides access to highly enantioenriched *C*-stereogenic, *P*-stereogenic as well as atropoisomeric molecules – key structural motifs in drugs and crop protection agents.

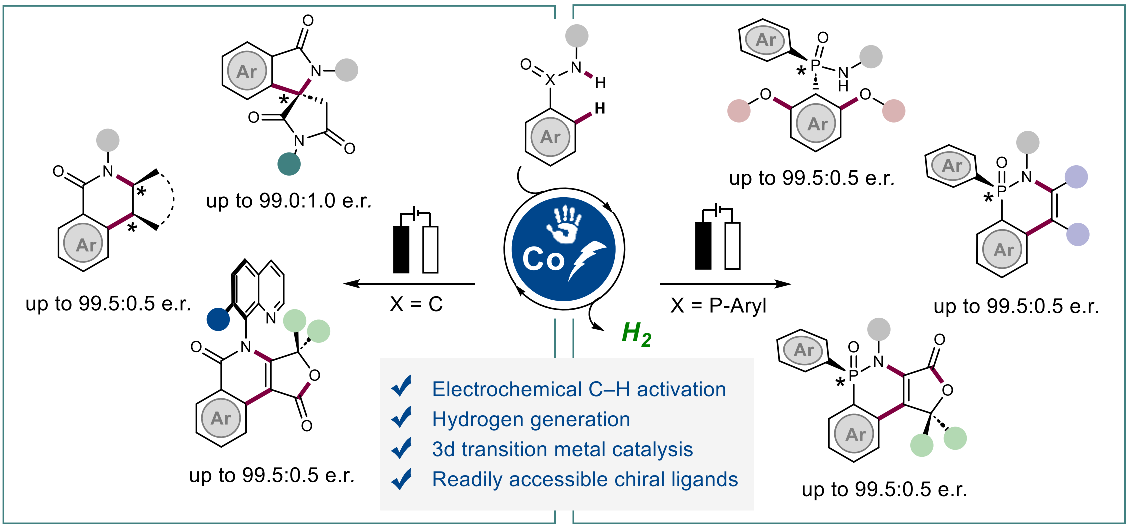

Figure 1: Enantioselective electrochemical cobalt-catalyzed C–H activation to access C-stereogenic, axially chiral, and P-stereogenic molecules.

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MPX_specDB: A FAIR Data Approach to Understanding Microplastic Pollution Through Spectroscopy

Robin Lenz [1], Franziska Fischer [1], Melinda Arnold [1], Verónica Fernández-González [2], Carmen María Moscoso Pérez [2], José Manuel Andrade-Garda [2], Soledad Muniategui-Lorenzo [2], Dieter Fischer [1]

[1] Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany
[2] University of A Coruña, Campus da Zapateira s/n, 15071, A Coruña, Spain

Microplastic pollution poses significant environmental challenges and requires innovative approaches for detection and characterisation. In this presentation, we present *MPX_specDB*, a comprehensive dataset of Raman and ATR-FTIR spectra of weathered and biofouled polymers. Originating from the JPI Oceans *microPlastiX* project, one of whose themes was the biofouling dynamics of plastic fragments, this dataset provides a resource for research on microplastic degradation and environmental impact. [1]

Micro-Raman and micro-FTIR have emerged as the most commonly applied techniques to characterise and quantify microplastic particles (MP). The analytical challenge is to sufficiently capture the wide range of materials, sizes and shapes, especially when samples have been exposed to environmental degradation, which changes their chemical fingerprints. Spectroscopic libraries used in MP analyses can benefit from the inclusion of polymer spectra weathered under different environmental conditions. In a coordinated marine mesocosm experiment we collected polymer samples weathered at several European coastal exposure sites, across seasons, in time series ranging from seven days to six months.

Data collection processes with changing contributors over time, measuring with different techniques, on different instruments, with the aim of providing a common data resource, can easily become a challenging reality in larger collaborative research projects. Our project was exactly in this position, and we show that data management according to the FAIR data principles [2] is the clear path to ensure transparency and understandability – not only for the wider community, but also within the project consortium. The talk will touch on lessons learned (e.g. naming conventions, reproducible data science scripts and interactive notebooks). We have leveraged open science tools to enhance accessibility, including an interactive data viewer and analysis web app. It allows researchers to explore spectra, filter data based on various parameters, and download relevant parts of the dataset for further analysis. The presentation will be complemented by a live demonstration of the application.

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O01

Lithium-Ion Battery Cell Identification with Magnetic Supraparticles

Sara Li Deuso [1], Simon Ziegler [2], Stephan Müssig [1], Florian Fidler [3], Daniel Haddad [3], Daniel Weber [3], Andreas Flegler [2], and Karl Mandel [1,2]

[1] Friedrich-Alexander-Universiät Erlangen-Nürnberg, Department of Chemistry and Pharmacy, Inorganic Chemistry, Erlangen, Germany
[2] Fraunhofer-Institute for Silicate Research ISC, Würzburg, Germany
[3] Magnetic Resonance and X-ray Imaging Department, Development Center X-ray Technology, Fraunhofer-Institute for Integrated Circuits IIS, Würzburg, Germany

The scarcity of resources used for lithium-ion batteries (LIBs) requires the development of suitable recycling technologies.[1] However, due to the lack of standardized cells and limited information regarding cell chemistry or respective components, recycling of LIBs is currently economically unviable.[2] Aiming to enable precise identification (ID) and associated with this tracking the origin of the cells, improving occupational safety and maximizing resource recovery, a possible solution is to equip LIB cells with a machine readable identifier. Particle-based tags with spectral encoding strategies, herein magnetic code-carrying supraparticles, have recently been introduced as an innovative technology for identifying even opaque materials, offering the opportunity to be incorporated into products,[3] such as battery cells.

In this contribution, it is demonstrated that supraparticles with defined magnetic ID codes can be integrated at different locations within LIB cells allowing the identification of un-opened, damaged or dismantled cells (Figure 1). Like a magnetic fingerprint, precisely tailored supraparticle structures facilitate their identification *via* magnetic particle spectroscopy (MPS) within seconds.[4] Aiming for applicability, strategies are proposed to meet the thermal and mechanical requirements of the integration positions, *e.g.* the pouch foil interface. Further, the impact of magnetic materials within battery cells on the magnetic ID code is investigated. In summary, these supraparticles pave the way to selectively mark and identify LIB cells, opening up the possibility of repair, recycling and reuse.

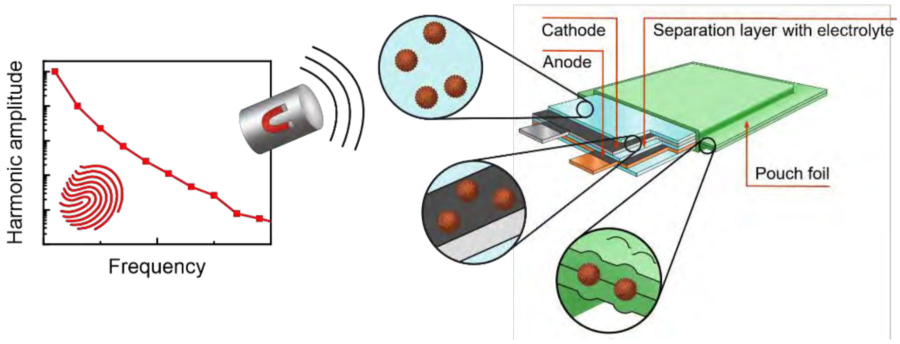

Figure 1: Equipping LIBs with magnetic code-carrying supraparticles.

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O02

Corrosion Behaviours of Current Collectors and Rechargeability of TiO_2 in Aqueous Electrolyte Aluminium-ion Batteries

Burcu Unal[1,2], Ozlem Sel[3], Rezan Demir-Cakan[1,2]

[1] Gebze Technical University, Department of Chemical Engineering, Kocaeli, Turkey
[2] Gebze Technical University, Institute of Nanotechnology, Kocaeli, Turkey
[3] Chimie du Solide et de l'Energie, UMR 8260, Collège de France, Paris, France

Lithium-ion batteries (LIBs) dominate the marketplace for portable devices and the electrical vehicles because of their highest energy densities. Some concerns about the use of highly flammable organic electrolytes, increasing demand, depletion of lithium reserves have been driving force for researchers to search alternative chemistries to compare with LIBs. Aqueous electrolyte aluminium systems (AAIBs) offer the potential to compete with LIBs, providing relatively low cost, high volumetric and gravimetric capacity, safety, abundant and ability to allow three electrons transfer. owever, the major disadvantage of AAIBs compared to non-aqueous batteries is the low energy density resulting from the low thermodynamic stability of water in the narrow potential window and problem of corrosion and hydrogen evolution reaction (HER) in current collectors arises, causing low discharge capacity and Coulombic efficiency.[1]

For these purposes, potential current collectors (titanium Ti, graphite plate GP, stainless steel SS and nickel Ni) were screened focusing on their corrosion behaviour and electrochemical stability.[2] Also TiO_2, as one of the most promising anodes, was synthesized to further emphasize the effect of current collector performance in 1.0 M $AlCl_3$ aqueous electrolyte. It has been proven by corrosion tests, cyclic voltammetry and charge-discharge studies that GP is the best current collector by minimizing the corrosion effect and HER.

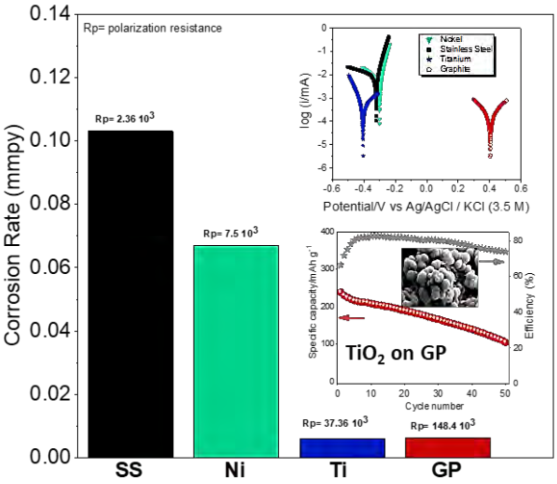

Figure 1: Current collectors corrosion behaviours and rechargeability of TiO_2.

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O03

Synthesis and Analysis of Hydroxyapatite-Based Biomaterials for Theranostic Applications

Natalia Charczuk [1], Sara Targońska [1,2], Agnieszka Śmieszek [3] and Rafal J. Wiglusz [1,4]

[1] *Polish Academy of Sciences, Institute of Low Temperature and Structure Research, Wroclaw, Poland*
[2] *Swedish University of Agricultural Sciences, Department of Molecular Sciences, Uppsala, Sweden*
[3] *University of Environmental and Life Sciences, Department of Experimental Biology, The Faculty of Biology and Animal Science, Wroclaw, Poland*
[4] *Silesian University of Technology, Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, Faculty of Chemistry, Gliwice, Poland*

Nanosized biomaterials based on synthetic hydroxyapatite (nHAp) exhibit similar properties to naturally occurring hydroxyapatite, a constituent of mammalian bones and teeth. nHAp finds broad applications in medicine, serving as a dental material or a composite base in implantology. Furthermore, in recent years, there has been intensive research into utilizing materials with an apatite structure in theranostics and bioimaging.

One of the key features that makes nHAp an attractive biomaterial is its ability to undergo ionic substitution within the crystal lattice. This substitution allows for the modification of biological properties as well as physicochemical characteristics such as morphology and surface properties. Substituent ions play a significant role in mineral homeostasis and the metabolic processes of cells and tissues surrounding implants. For instance, the introduction of silicate groups (SiO_4^{4-}) leads to an enhanced response from osteoclasts and osteoblasts, alongside improved biocompatibility. Furthermore, doping with lithium ions (Li^+) increases osteogenesis and the mechanical strength of implants, while rare earth ions such as europium(III) and gadolinium(III) ions (Eu^{3+} and Gd^{3+}) enable the attainment of luminescent and magnetic properties.

The physicochemical studies of co-doped nanosized hydroxyapatites with Li^+, Eu^{3+}, Gd^{3+}, and SiO_4^{4-} ions primarily rely on XRDP and FT-IR analyses, and optical characteristics. Additionally, microscopic methods such as SEM-EDS, HR-TEM, surface analysis using BET, and zeta potential measurements are used. Combined with biological studies, these approaches help to assess the material's potential applications. The current work presents a comprehensive analysis of nHAp 'step by step' — from synthesis to establishing its biocompatibility and its capability for simultaneous cell/tissue treatment and *in vivo* imaging.

O04

Casein-coated magnetic nanoparticles for controlled drug release

Nils Meier [1], Christina Wenck [1], Alexander-Nicholas Egler-Kemmerer [1], Frank Wiekhorst [2], Regina Bleul [1]

[1] Fraunhofer Institute for Microengineering and Microsystems IMM,
Carl-Zeiss-Straße 18-20, 55129 Mainz, Germany
[2] Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin, Germany

Magnetic nanoparticles (MNP) have been intensively studied in the biomedical field. They can be used as biosensors, for magnetic resonance imaging (MRI), for magnetic particle imaging (MPI) or as a hyperthermia treatment in cancer therapy. However, often they exhibit low stability in physiological medium or toxicity in such applications. Thus, a surface modification of the MNP is applied to enhance their stability and biocompatibility.[1] Casein is an abundant, amphiphilic protein that has unique drug release capabilities especially for hydrophobic or poorly soluble substances.[2] In this study we present the continuous production of iron oxide nanoparticles and their subsequent surface modification with casein as hydrophobic release layer.

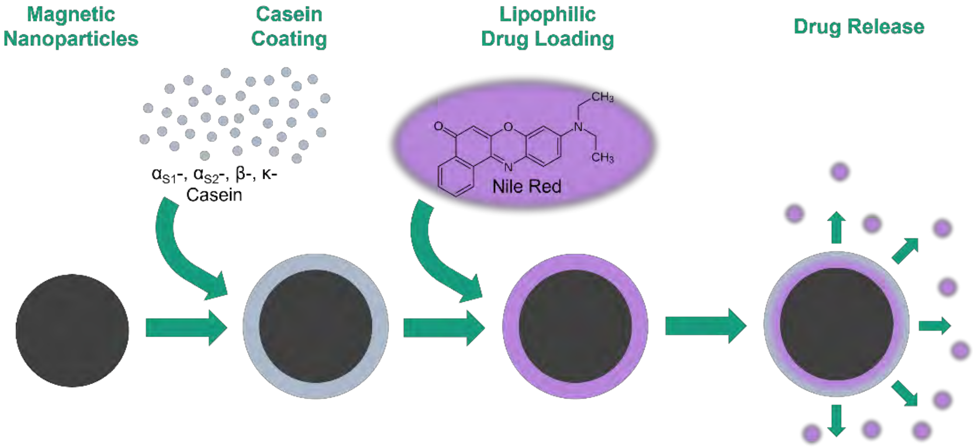

Figure 1: Illustration of MNP modification, drug loading and release.

The MNP were continuously produced by alkaline precipitation in a micromixer set-up and preliminary stabilized with tannic acid.[3] After magnetic separation the MNP were coated with different forms of casein (Na-caseinate and casein micelles) to improve their stability and further functionalize them with a hydrophobic release layer.

The casein coated MNPs have been thoroughly investigated for their improved stability, magnetic behavior, and drug release properties. A lipophilic dye could successfully be loaded into the casein layer and continuously be released in physiological medium, without precipitation of the MNP. With the possibility of tracing the MNP with MPI and simultaneously releasing a pharmaceutical substance a huge step towards a theragnostic anti-cancer agent was made. Induced release by hyperthermia will be the focus of future studies.

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O05

Identification and structural optimization of a core-independent carboxamide chemotype as novel *P. falciparum* inhibitors

Alicia Wagner [1], Roger Trombley [1], Maris Podgurski [1], Jacqueline Smith [1], Meng Cui [2], Adriana A. Marin [3], Edward Yu [4], Steven P. Maher [3], Dennis E. Kyle [3], Roman Manetsch [1,2]

[1] Northeastern University, Department of Chemistry and Chemical Biology, Boston, United States of America
[2] Northeastern University, Department of Pharmaceutical Sciences, Boston, United States of America
[3] University of Georgia, Center for Tropical and Emerging Global Diseases, Athens, United States of America
[4] Case Western Reserve University, Department of Pharmacology, Cleveland, United States of America

The recent rise in drug resistance against current malaria treatment options necessitates the identification of alternative malaria targets and new antimalarial drugs. *Plasmodium falciparum* formate-nitrite transporter (*Pf*FNT), a lactic acid efflux pump, has been identified as one such druggable target,[1–3] though the current inhibitor class is not drug-like as substrates possess a PAINs moiety.[4–5]

Through a virtual high-throughput screen (vHTS), cheminformatics-driven down selection, and structure activity relationship (SAR) studies, we have identified a 1,2,4-triazole-containing carboxamide scaffold; while the most promising triazole displayed 519-nM potency against the asexual blood stages of the parasite, this activity was unable to be surpassed. Scaffold hopping efforts then revealed six alternative cores with up to a 31-fold increase in potency from the aforementioned frontrunner triazole. Further modifications to the molecule periphery have enabled the identification of numerous molecules with single-digit nanomolar potency. Phenotypic assays have suggested hits are on target through a decrease in intracellular pH when compounds are added to live trophozoites, one of the asexual blood stages of the parasite. *In vivo* studies are underway for several current front-runners and additional structure-activity and structure-property relationship studies are ongoing to further optimize this promising new chemotype.

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Cleaning (waste)water using biowaste materials like spent coffee

Inga Block [1], Andreas Taubert [1]

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

On average the german coffee drinker consumes 3.4 cups of coffee a day, producing ca. 43 g of spent coffee grounds (SCG) daily.[1] Typically, these are discarded as (bio)waste. Our group focuses on giving SCGs and other biowaste products a new purpose as filter materials for the filtration and cleaning processes of wastewater.[2,3] For this purpose, we carbonize our SCGs using a rather simple pretreatment and carbonization step.

We found a way to produce carbonaceous materials from SCGs, which would otherwise be discarded as biowaste, using a rather simple pretreatment and carbonization step. Different precursors added to the SCGs enable the adjustment of surface areas, pore sizes and other properties influencing the adsorption capacities of the new activated carbons (AC). In addition, we are looking into making the ACs magnetic, with the goal of simplifying filtration and recycling processes. Adsorption experiments are carried out on several organic contaminants often found in wastewaters, eg. diclofenac, tetracycline and bisphenol A, in single studies as well as in mixed systems.

The gained carbons show high adsorption capacities and removal efficiencies for all systems proving the suitability of these materials for water filtration. Hence, SCGs present a promising alternative route for the synthesis of ACs used in (waste)watertreatment.

Figure 1: Filtration of organic contaminants out of water using activated carbon (AC) generated from spent coffee grounds (SCG)

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O07

How do Sb(V) corroles sensitize singlet oxygen? A spectroscopist's tale

Volkan Caliskanyürek [1], S. Eulberg [2], O. Lange [1], M. Bröring [2], S. Tschierlei [1]

[1] Department of Energy Conversion, Institute of Physical and Theoretical Chemistry, TU Braunschweig

[2] Institute of Inorganic and Analytical Chemistry, TU Braunschweig

Singlet oxygen ($^1O_2$) is a highly reactive species crucial in diverse chemical reactions, especially in the photooxidation of organic molecules to yield peroxides and diketones. It is also utilized in photodynamic therapy (PDT) for effective anti-cancer treatment. In the laboratory, the generation of $^1O_2$ is achieved through the use of photosensitizers (PS) that sensitize triplet oxygen ($^3O_2$), allowing for controlled and targeted applications. In this context, we present three different Sb-based dihalide-corrole complexes that not only respond to visible light (λ > 400 nm), but also exhibit a singlet oxygen quantum yield $\Phi_{^1O_2}$ exceeding 95%.

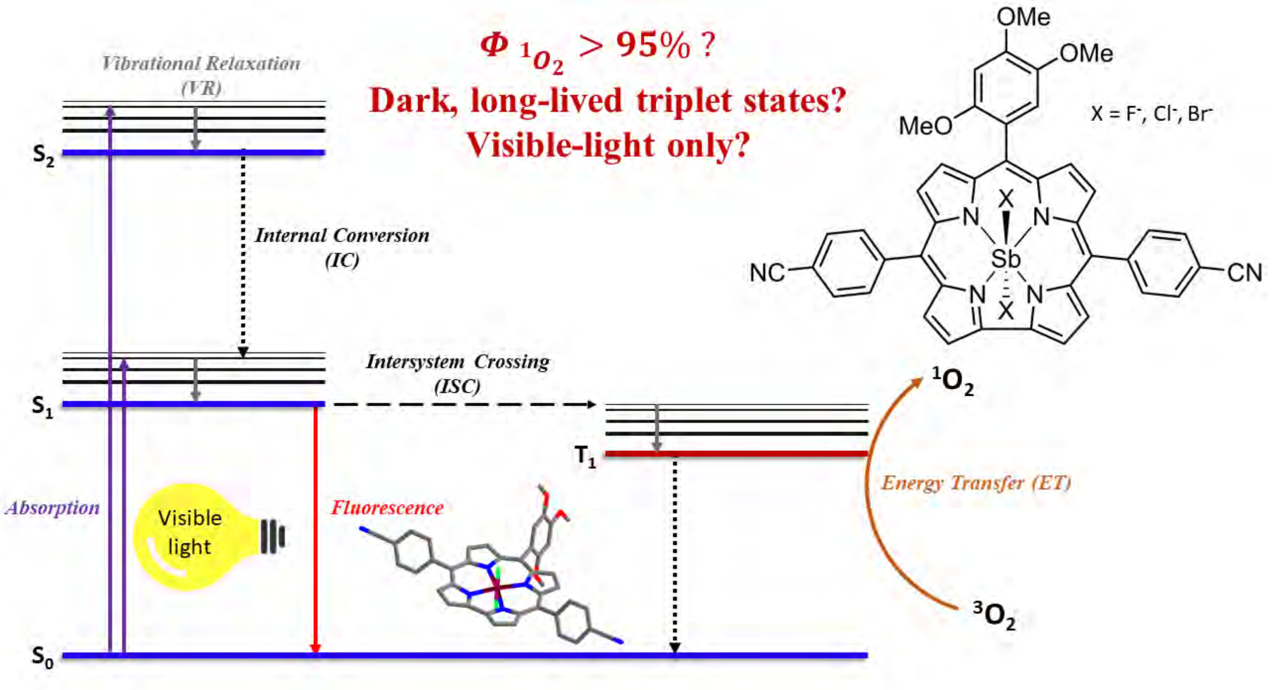

Figure 1: Structure of Sb(V) corroles and a Jablonski scheme presenting one pathway to generate $^1O_2$.

Therefore, the talk explores the intriguing interaction between the essential axial ligands (X = F^-, Cl^- or Br^-) in relation to their remarkable impact on the photophysical properties and the efficiency of $^1O_2$ sensitization. In addition to our spectroscopic and photocatalytic findings, TDDFT calculations are used to provide a comprehensive explanation of the involvement of axial ligands in catalytic reactions and the generation of singlet oxygen.

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O08

Strategies to break the C_3-symmetry of tris(amido)amine ligands

Marilyn Naeem [1], David R. Manke [1]

[1] *University of Massachusetts Dartmouth, Massachusetts, United States of America*

Tuning the local environment around a metal center controls its reactivity, allowing for thermodynamic and kinetic control in catalysts. Beyond the primary coordination sphere, control of the residues at a distance outside the range for metal coordination (the secondary coordination sphere) can have significant impact on the binding and reactivity of substrates, controlling substrate orientation, facilitating proton and electron transfer, etc. The tris(amido)amine, or tren, scaffold is a well-recognized C_3-symmetric, trianionic, tetradentate ligand set. The development of new strategies to break the C_3 symmetry of this ligand set allows the scope of trens to be expanded; this gives the option to change symmetry from C_3 to C_S, the charge of the ligand set, the directional steric impact of the ligand, the electron donation of the system, and the ability to provide multiple secondary coordination sphere functionalities in a single ligand. The syntheses, spectroscopic characterization, and reactivity of a new series of tren-based ligands is discussed. This flexibility of the ligand scaffold through two novel symmetry-breaking mechanisms have been demonstrated based on both carbon-nitrogen coupling and copper (II) catalysis, characterized by NMR and X-ray crystallography.

O09

Communicating the future of Chemistry – Science Communication

Samuel Van Gele [1]

[1] *Nanochemistry Department, Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany*

Chemists are pioneers responsible of pushing forward the frontier of knowledge. New innovative chemicals, materials and technologies are paving the way to a greener and more sustainable future for society. However, the potential of these advancements is often obscured in public discourse due to the communication gap between scientists and the general public.

The art of effectively communicating scientific research to a broader audience is not just an add-on but a fundamental aspect of fostering a meaningful dialogue about scientific advancements. How scientists communicate their research to a broader audience is of prime importance to foster discussion about and trust in science.[1,2]

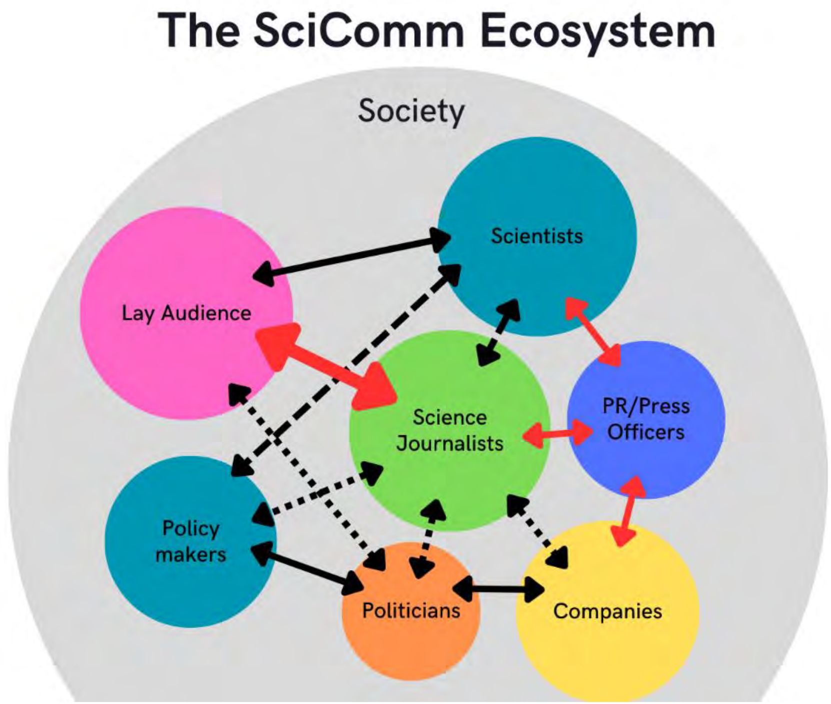

Figure 1: The simplified Science Communication Ecosystem

The science communication ecosystem is complex and consists of many actors interplaying, each with their own stakes and agenda. Understanding this ecosystem is the first step to shape how we will communicate the greener future of chemistry to society on a whole.

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O10

Tetraoxa[8]circulenes – A Platform for Polymers and Frameworks

Patrick W. Fritz [1], Tianyang Chen [2], Mircea Dinca[2], Ali Coskun [1]

[1] University of Fribourg, Department of Chemistry, Fribourg, Switzerland
[2] MIT, Department of Chemistry, Boston, USA

Tetraoxa[8]circulenes (TOCs) are a subclass of hetero[X]circulenes that have seen considerable interest from the computational community due to their aromatic motifs and from experimentalists due to their electronic properties. (*1, 2*) Despite that, only a few small-molecule TOCs have been reported in the literature, while extended structures such as polymers or framework materials were missing completely.

In 2022, we reported the first extended polymeric TOC (pTOCs) based on a Lewis acid-mediated cyclization procedure.(*3*) The obtained polymers featured tunable porosity and could be post-synthetically doped to tune their semiconducting properties. Based on these findings, we developed new protocols for synthesizing pTOCs. We obtained a system with crown ether-like pores capable of selectively capturing Li-ions from complex mixtures (Na^+, Ca^{2+}, Mg^{2+}, …) and were able to leverage it for the recycling of used energy storage devices of various electrode chemistries (LiS, Li-ion, and Li-metal).

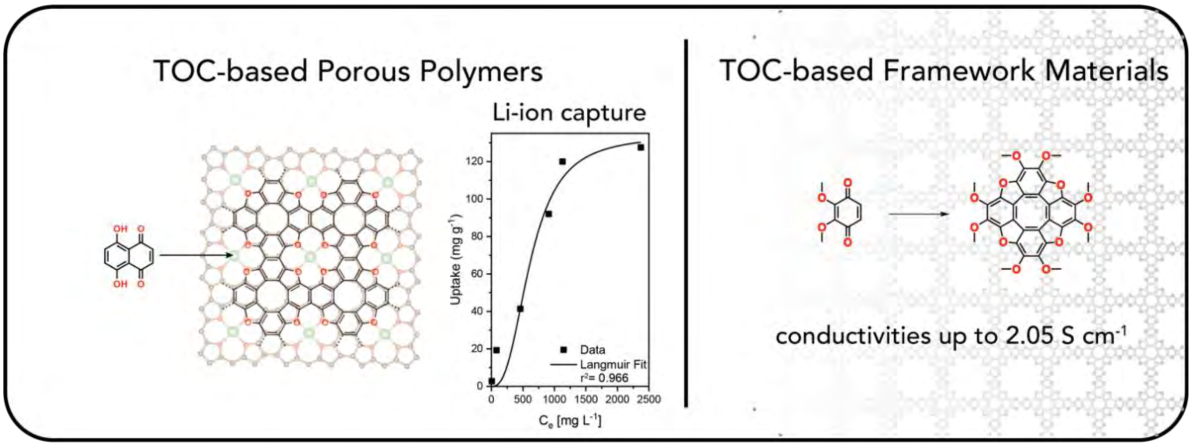

Figure 1: TOC-based porous polymers and precursors for framework materials.

The biggest drawback of pTOCs are their anisotropic properties. Framework-type materials could solve these problems, however, the preparation of functionalized TOC precursors beyond alkylation or *π*-extension had not been realized. To that end, we have developed a synthetic protocol toward an hydroxy-functionalized TOC precursor and have used it for the synthesis of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs). While the framework chemistry of the fully organic systems resulted in poor semiconductors, the TOC-based MOFs showed exceptional conductivities of up to 2.05 S cm^{-1} enabling their use as chemical sensors or as active materials in energy storage devices.

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O11

Bimetallic MnRu nanoparticles immobilized on supported ionic liquid phases (Mn_xRu_{100-x}@SILP) for selective hydrogenation reactions

Johannes Zenner [1,2], Liqun Kang [1], Serena DeBeer [1], Alexis Bordet [1], and Walter Leitner [1,2]

[1] Max Planck Institute for Chemical Energy Conversion, 45470 Mülheim, Germany
[2] RWTH Aachen University, Institute for Technical and Macromolecular Chemistry, 52074 Aachen, Germany

Selectivity control in hydrogenation is of crucial importance to maximize process efficiency while minimizing the amount of waste, in particular when considering a transition toward a sustainable chemical industry.[1–2] In this context, bimetallic nanoparticles combining noble metals with their base metal 3d congeners (e.g. FeRu, CoRu, CoRh, CuPt or FePt) have proven to be particularly effective hydrogenation catalysts due to their versatility, the potential synergistic effects arising from the combination of different metals, and their capacity to activate H_2 in various modes. [2–3] Although Mn is abundant in nature and has a low environmental impact, the preparation and application of similar materials containing Mn as 3d metal has received far less attention thus far.

Herein, we report the synthesis of bimetallic MnRu nanoparticles on an imidazolium-based supported ionic liquid phase (Mn_xRu_{100-x}@SILP, Figure 1a) following an organometallic approach. The materials were characterized (e.g. by electron microscopy and X-ray absorption spectroscopy) and applied in the hydrogenation of benzylideneacetone as a model reaction. It could be demonstrated that the Mn:Ru ratio has a crucial influence on the catalysts' activation mode of H_2, making it possible to target different hydrogenation products with high selectivity (Figure 1b).

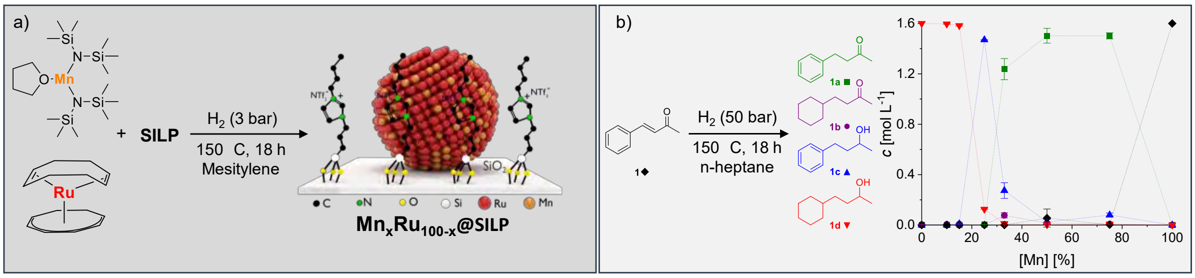

Figure 1: a) Synthesis of Mn_xRu_{100-x}@SILP and b) variation of the Mn:Ru ratio in the hydrogenation of benzylideneacetone.

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O12

The Art of Selectively Removing Electrons from Organ(ometall)ic Molecules and Elements in Condensed Phase

Malte Sellin [1], M. Seiler [1], T. Heizmann [1], J. Fischer [1], J. Willrett [1], Ingo Krossing [1]

[1] *University of Freiburg, Institute of Inorganic and Analytical Chemistry, Freiburg, Germany*

The removal of an electron from a molecule (one-electron oxidation/ deelectronation) is one of the most fundamental chemical reactions at all. This reaction however leads in the most cases to reactive radical-cations, which are often difficult to handle in condensed phase. The handling not only requires both sufficiently weakly coordinating anions (e.g. perfluorinated alkoxyaluminates) and solvents (e.g. fluorinated benzenes), but also the right reagents for removing the electron.

Typical inorganic oxidants e.g. Ag^+ and $[NO]^+$ often tend to react in unwanted side-reactions instead of a deelectronation with challenging substrates.[1] Perfluorinated arenes such as naphthalene^F, anthracene^F and phenanthrene^F can be reversibly deelectronated and isolated as $[F\{Al(OR^F)_3\}_2]^-$ ($OR^F = OC(CF_3)_3$) salts.[2–4] These innocent deelectronators distribute the radical-cationic charge over a large π-system and prevent with that side reactions, while having very strong redox potentials up to 2.0 V vs. $Fc^{+/0}$. Both the selectivity and the potential of the perfluoroarenium radical-cations have been proven by reaction with arenes, metal carbonyls, other transition metal complexes and (non)metals (Figure 1).[2,4,5]

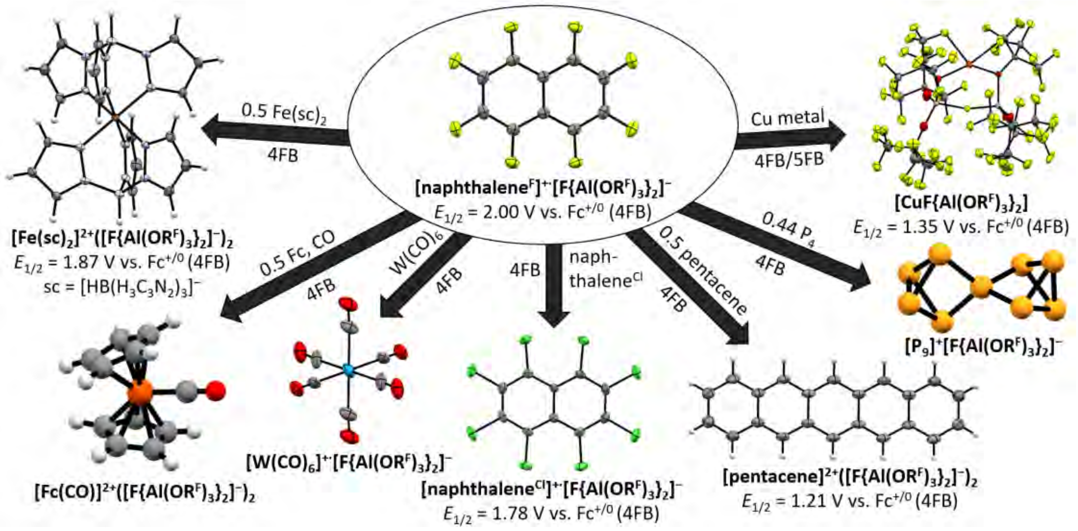

Figure 1: Scope of the perfluoronaphthalenium radical cation deelectronator.

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O13

Cyclopentadienone Iron Complexes derived from Diaminoacetylenes as Efficient Hydrogenation Catalysts

Lukas Körner [1], Ludwig Hackl [1], Dirk Bockfeld [1], Matthias Tamm* [1]

[1] *Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig*

The reactivity of electron-rich diaminoacetylenes (DAAs) is driven by their "hidden diaminodicarbene character", which enables versatile transformations.[1] In the past, we showed for instance the thermal dimerization and subsequent cyclization to strong σ-donor cyclic bent allene (CBA) ligands.[2] In contrast, a proton-induced dimerization followed by oxidation led to the first fully characterized cyclobutadiene dication, whose aromaticity was evaluated by detailed computational methods.[3] Our current research interest is focused on the synthesis and application of amino-substituted cyclopentadienone (CPD) iron complexes. Symmetric as well as asymmetric tetraamino-CPD iron tricarbonyl complexes can be obtained from DAAs and $Fe(CO)_5$ *via* a unique ferracyclobutenone intermediate (Scheme 1).[4] Diaminodiaryl substituted CPD iron tricarbonyl complexes are accessible from the free CPD ligands, which are synthesized from DAA and cyclopropenone. The transformations into dicarbonyl acetonitrile complexes provide highly active precatalysts which hydrogenate a variety of ketones in the presence of H_2 at low overpressures (3 bar) at room temperature or with isopropanol at 80 °C in 2h, both with low catalyst loadings of 1-2 mol%. Additionally, the electron rich CPD iron catalysts have been investigated in catalytic reductive amination reactions revealing high activity, especially compared to non-nitrogen substituted congeners, and chemoselective reactivity.

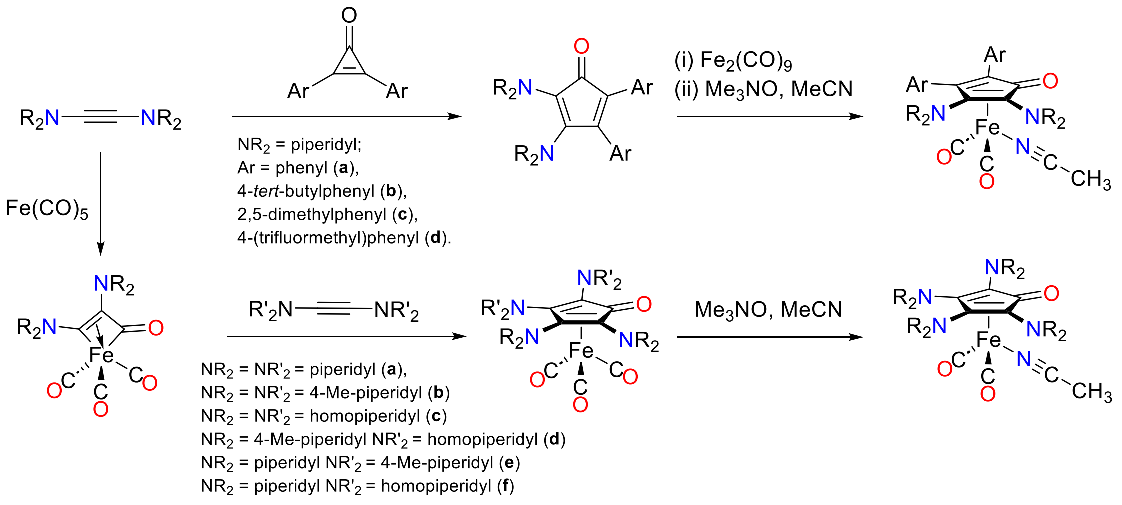

Figure 1: Synthesis of tetraamino and diamino CPD iron precatalysts starting from diaaminoacetylenes.

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O14

Decarboxylative Glaser Coupling of Aryl Propiolic Acids

Lena Viergutz [1], Huihui Kong [2], Lacheng Liu [3,4], Alexander Sandvoß [1], Xinchen Peng [2], Henning Klaasen [1], Harald Fuchs [3,4], Armido Studer [1]

[1] *Universität Münster, Organisch-Chemisches Institut, 48149 Münster, Germany*
[2] *Nanjing University, Herbert Gleiter Institute of Nanoscience, Nanjing 210094, P. R. China*
[3] *Universität Münster, Center for Nanotechnology, 48149 Münster, Germany*
[4] *Universität Münster, Physikalisches Institut, 48149 Münster, Germany*

On Surface Chemistry has attracted extensive attention as a bottom up strategy for the synthesis of two-dimensional materials with potential interesting properties and functions. Various organic reactions have been realized on metal surfaces.[1,2]

The Glaser coupling[3] is the most promising approach for the preparation of extended single-layered graphdiyne nanolayers. Moreover, it is one of the most heavily used on-surface reactions.

On-surface decarboxylation of aryl carboxylic acids leads to fragmentation of gaseous CO_2, which results in Ullmann type couplings.[4] Decarboxylative Glaser coupling of aryl propiolic acids was realized on a silver surface leading to poly(diynes) (Figure 1). In comparison with the "classical" *on-surface* Glaser coupling, defects of the resulting poly(diynes) were reduced to a minimum and the polymer length was increased.

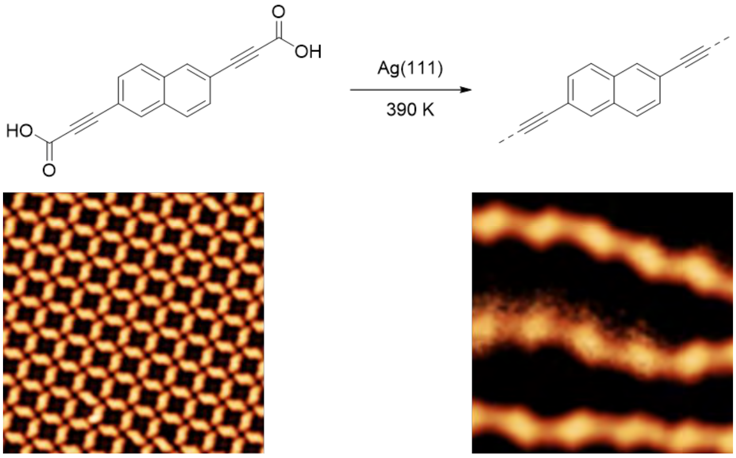

Figure 1: Brutto reaction equation of the decarboxylative Glaser coupling of an aryl propiolic acid and STM images of the nanostructures on Ag(111) before and after the reaction.

Additionally, the new functionality is compatible with aryl bromide functionalities. The formation of asymmetric metal-organic polymers in high selectivity by a chemoselective sequential reaction was achieved. DFT calculations and STM simulations support the correct structural assignment.

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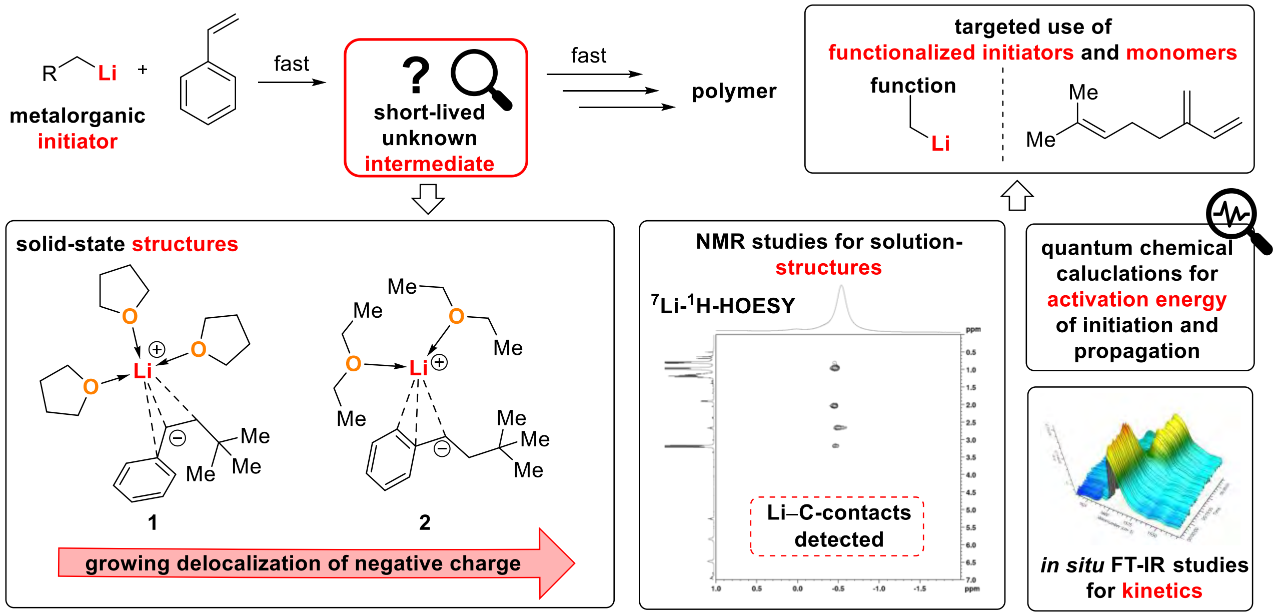
O15

Rethinking Anionic Polymerization Towards a Greener Future

Annika Schmidt[1], Bastian Grabe[1], Wolf Hiller[1], Carsten Strohmann[1]

[1] *TU Dortmund University, Faculty of Chemistry and Chemical Biology, Dortmund, Germany*

Carbometallation reactions display one of the classical reactivities of metalorganic compounds and play a major role in applications like anionic polymerizations. Despite their long history in academic research and high industry relevance,[1] the mechanism of anionic polymerization and the underlying carbometallation steps has not been fully explained, *inter alia*, due to the inability to capture the active intermediate species from the fast polymerization reaction.[2] To understand the structure-reactivity relationship[3] of the short-lived active anionic polymer chain, the first intermediate carbometallation product of anionic styrene polymerization was synthesized selectively and crystallized with various ligands, like thf (**1**) and diethyl ether (**2**). The solid-state structures obtained by X-ray diffraction indicate different coordination patterns that have also been examined in solution with help of additional NMR experiments. Through *in situ* FT-IR studies solvent-dependent reactivities have also been elucidated that may be explained *via* quantum chemical calculations. With this precise understanding of the short-lived intermediate and its reactivity, anionic polymerizations are aimed to be controlled in a more precise way to insert bio-compatible functionalizations in anionic initiators, to promote recyclability or to transfer the obtained findings on different bio-based double-bond containing monomers (e.g. myrcene).



Scheme 1: Solid state structures and further analytics of first carbometallation intermediates.

References:

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FUTURESILIENCE
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P001

Nano vs. Bulk – Surfactant-controlled Photophysical and Morphological Features of Luminescent Lanthanide MOFs

Moritz Maxeiner [1], Lea Wittig [1], Alexander Sedykh [1], Thomas Kasper [1], Klaus Müller-Buschbaum [1]

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

Over the past twenty years, there has been extensive research on metal-organic frameworks (MOFs) due to their capacity to integrate molecules and ions within the voids of their 3D crystal structure. The π-system inherent in organic linkers allows for light absorption in the UV-spectrum, rendering them effective sensitizers for lanthanide (Ln) photoluminescence. This property endows lanthanides with exceptional phosphorescent characteristics, among their various advantages.[1]

This study utilized a series of organic linkers (H_2bdc, H_2bpdc, and H_2bpydc) in conjunction with trivalent lanthanides (Ln^{3+}= Eu^{3+}, Tb^{3+}) during synthesis and post-synthetic modification, employing surface-active agents (CTAB, PVP) to assemble luminescent nMOFs across three archetype MOFs: nLn^{3+}-bdc, nDUT-5:Ln^{3+}, and nMOF-253:Ln^{3+}. The controlled bottom-up particle downsizing resulted in improved dispersibility and morphology, achieving particle sizes as small as 35 nm with narrow size distributions of ±5 nm, 21-fold smaller than their bulk counterparts. Additionally, impressive luminescence QYs of up to 78.1(3)% for solid-state are demonstrated. Further photophysical attributes, such as energy transfer, are also notably influenced by particle size, surfactant composition, and post-synthetic modifications.[2]

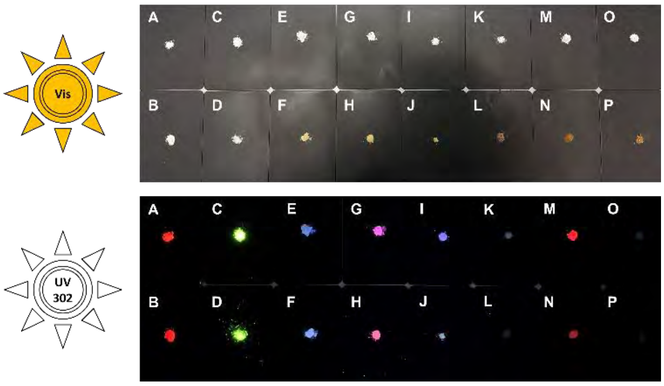

Figure 1: Investigated bulk MOFs and nMOFs exposed to Vis- and UV-light. A=Eu^{3+}-bdc, B=nEu^{3+}-bdc, C=Tb^{3+}-bdc, D=nTb^{3+}-bdc, E=DUT-5, F=nDUT-5, G=DUT-5:Eu^{3+}, H=nDUT-5:Eu^{3+}, I=DUT-5:Tb^{3+}, J=nDUT-5:Tb^{3+}, K=MOF-253, L=nMOF-253, M=MOF-253:Eu^{3+}, N=nMOF-253:Eu^{3+}, O=MOF-253:Tb^{3+}, P=nMOF-253:Tb^{3+}.

Ultimately, this research aims to comprehensively elucidate the distinctive properties of nMOFs in comparison to their bulk counterparts. Given the crucial role of surfactants in this synthesis process, the advantages and limitations of this approach were thoroughly evaluated concerning various features of nMOFs.

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P002

Investigation of the influence of lanthanide ions on the spectroscopic properties of mixed orthovanadate systems

Aleksandra Bartkowiak [1], Adam Watras [1], Marta Kardach [1], Paulina Sobierajska [1],
John M. Reeks [1], Philippe Boutinaud [2] and Rafal J. Wiglusz [1,3]

[1] Institute of Low Temperature and Structure Research Polish Academy of Sciences, Wroclaw, Poland

[2] Université Clermont Auvergne, Clermont Auvergne INP, CNRS, ICFC, Clermont-Ferrand, France

[3] Silesian University of Technology, Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, Faculty of Chemistry, Gliwice, Poland

Orthovanadate materials doped with lanthanide ions have demonstrated significant potential in various fields of applications, including sensors, light-emitting diodes, bioimaging, lasers, and more.[1] Similarly, YXO_4 structures (where X = As^{5+}, Cr^{5+}, P^{5+}, or V^{5+}) have been receiving much attention in the scientific community on account of their advantageous characteristics, such as photodegradation resistivity and high thermal stability.[2]

The objective of this study is to examine how the presence of lanthanide ions affects the spectroscopic properties of $YV_{1-z}X_zO_4$ systems. In these mixed orthovanadate structures, V^{5+} ions are substituted with P^{5+} and/or As^{5+} ions. This replacement results in a significant structural disorder that influences the spectroscopic properties of $YV_{1-z}X_zO_4$ nanosized materials doped with lanthanide ions. The nanomaterials were synthesized using various techniques, including sol-gel, hydrothermal, and precipitation methods. Additionally, their structural and physicochemical properties were analysed using XRD, SEM, ICP, and spectroscopic measurements.

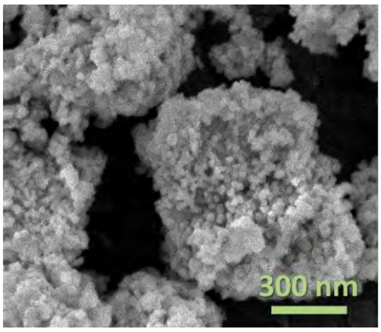

Figure 1. SEM image of YXO_4 nanomaterials doped with lanthanide ions.

The authors acknowledge the National Science Centre Poland (NCN) within the project: 'Preparation and modulation of spectroscopic properties of $YXZO_4$, where X and Z − P^{5+}, V^{5+}, As^{5+}, doped with "s^2-like" ions and co-doped with rare-earth ions' (UMO-2019/33/B/ST5/02247).

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P003

SYNTHESIS AND CHARACTERIZATION OF TETRA OR OCTA 7-ALKOXY-2-NAPHTHOXY SUBSTITUTED METAL AND METAL-FREE PHTHALOCYANINES

Sena AKBULUT [1], Zafer ODABAŞ[1]

[1] *Marmara University, Institute of Science, İstanbul, Turkey*

Although Phthalocyanines (Pcs) and metal complexes are organic compounds, they have organic, inorganic, physical and electrochemical properties that attract interdisciplinary interest thanks to their metal retention properties. Pcs have a ring with 18π electrons. Dozens of different metals can be bonded to this ring, and the bonded metals can change the properties of the compound. Moreover, the environment of the ring (peripheral or non-peripheral region) can be modified with different organic groups and show their own characteristic properties.[1]

Chemical structures and electrical, spectroscopic and electrochemical properties of Pcs; The substituents in the peripheral and non-peripheral positions and the metals bonded in the center can be changed and their usage areas can be expanded by synthesizing Pcs with different properties.[2] At the same time, different properties can be provided to Pcs by using different connection bridges (oxo, azo, thio, imine) and can contribute to the formation of their characteristic properties.[3] Although Pcs are generally synthesized with oxo bridges, they can also be synthesized with azo, thio and imine bridges. Thanks to these properties, countless original phthalocyanines with different physical and chemical properties and different usage areas can be synthesized, which makes phthalocyanine very interesting among scientists and the subject of many studies.

In this study, first of all, 7-alkoxy-2-naphthol substance; Different starting compounds were obtained by reacting with 3-nitrophthalonitrile, 4-nitrophthalonitrile and 4,5-dichlorophthalonitrile, and it was aimed to synthesize and characterize oxo-bridged metal and metal-free phthalocyanine. Novel Pc compounds were synthesized, purified, their structures were elucidated by classical spectroscopic methods, and their physical, chemical and spectrochemical properties were investigated, contributing to the literature and a study that would guide Pc scientists.

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P004

Quantum Chemical Characterization of Palladium(II) and Platinum(II) metallopnictinidenes

Nils Wegerich [1], Marc C. Neben [2], Tarek Al Said [3], Hendrik Verplancke [1],
Serhiy Demeshko [2], Alexander Schnegg [3], Sven Schneider [2], and Max C. Holthausen [1]

[1] Goethe University, Institute of Inorganic and Analytical Chemistry, Frankfurt, Germany
[2] Georg-August-University, Institute of Inorganic Chemistry, Göttingen, Germany
[3] MPI for Chemical Energy Conversion, Mülheim an der Ruhr, Germany

Subvalent organic Nitrenes (N–R) are key intermediates in nitrogen transfer reactions.[1,2] The relative triplet-singlet energy difference mainly determines their reactivity.[3] Heavier pnicitinidene analogues are also of increasing interest, as they could potentially be used as pnictogen building blocks in future synthesis strategies. However, such reactions have hardly been investigated so far.[4–6] Paramagnetic Pd(II) and Pt(II) metallonitrene complexes synthesized by the Schneider group exhibit unexpectedly low zero field splittings indicating small spin-orbit coupling contributions despite the presence of heavy transition metal atoms.[7,8] Here, we report the quantum chemical examination of electronic structures and magnetic properties of a series of Pd(II) and Pt(II) metallopnictinidenes (M–Pn; Pn = N, P, As, Sb, Bi). Our investigations demonstrate how the spin density distribution between the transition metal atom and pnictinidene ligand determines the extent of the zero field splitting.

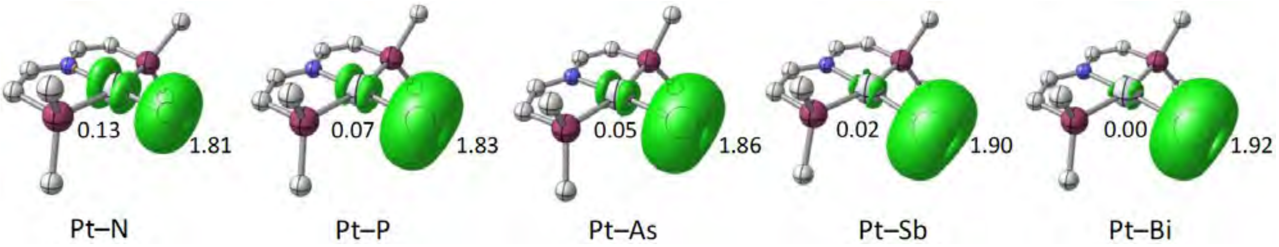

Figure 1: Spin density plots of Pd(II) and Pt(II) metallopnictinidenes. Natural spin populations of the transition metal atom and the pnictinidene ligand are given for each complex. For clarity, H atoms are omitted, and only tertiary C atoms of t-Bu groups are shown.

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P005

Synthesis and Reactivity of Fluorinated Terphenyl Nitrenes in Cryogenic Matrices

Maurice Niehoff, Julien F. Rowen, Wolfram Sander

Ruhr-University Bochum, Faculty of Chemistry and Biochemistry, 44801 Bochum, Germany

Nitrenes are reactive intermediates with a short lifetime at ambient conditions due to their electron deficiency. They exhibit a robust triplet ground state and are of considerable interest in chemistry especially for reaction mechanisms and the construction of organic magnetic materials.[1] The aim of this work is to design kinetically stabilized, terphenyl-based triplet nitrenes and investigate solvation effects on these inside cryogenic matrices.[2]

The parent *m*-terphenyl azide as well as two fluorinated derivatives **1a** and **1b** were synthesized and deposited under matrix isolation conditions in Ar at 3 K. Upon UV irradiation, triplet nitrenes **2a** and **2b** are generated and characterized by IR and UV spectroscopy. Secondary photochemistry of nitrenes **2a** and **2b** with 365 nm leads to the corresponding azirines **3a** and **3b**. In contrast to these findings, the parent *m*-terphenyl azide shows a complex photochemistry with a product ratio depending on the host gas. Analogue experiments in KBr matrices allowed to monitor the thermal decay of the nitrenes up to room temperature. Nitrenes **2a** and **2b** were found to persist in KBr matrices up to 70 and 120 K, respectively. At higher temperatures, a complex product mixture is obtained. Overall, cryosolvation effects on terphenyl-based nitrenes were observed and their lifetime extended in KBr matrices beyond cryogenic conditions.

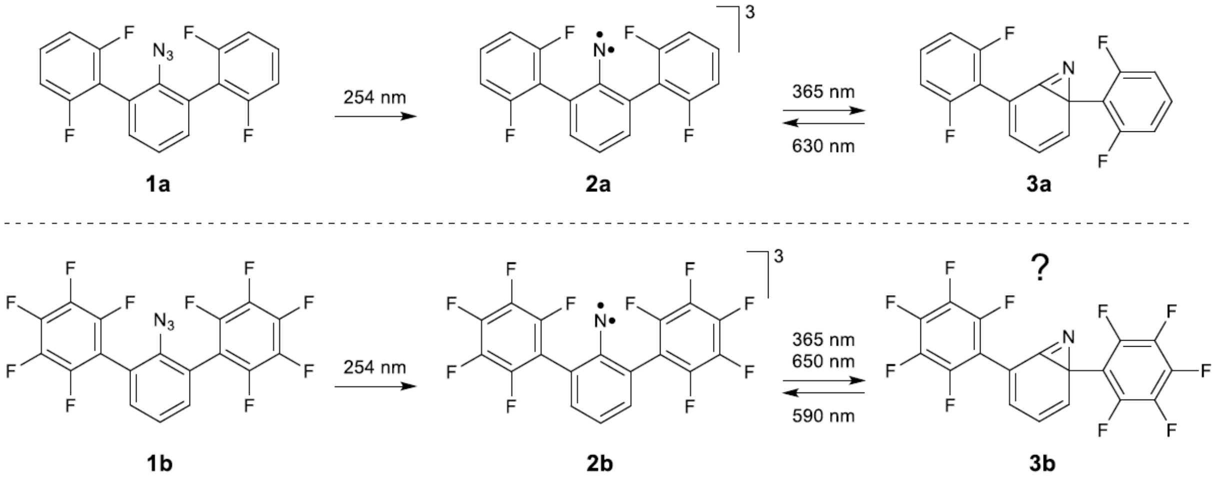

Figure 1: Photochemical synthesis and rearrangement of tetrafluoro and decafluoro terphenyl nitrene.

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P006

Selective Monoarylation of Ammonium Triflate with Aryl Chlorides Catalyzed by [Pd(β-MeNAP)Br]$_2$ and AdBrettPhos

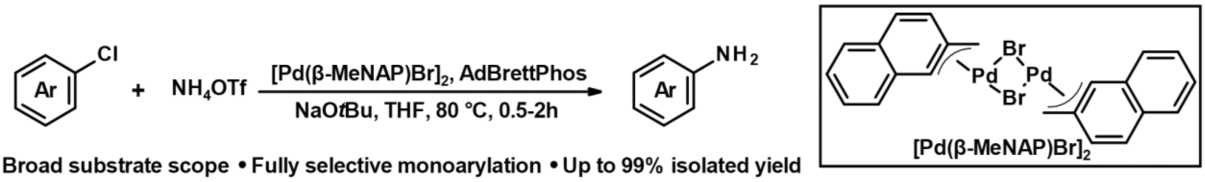
Bingxiang Xue [1], Jie Shen [1], Sourav Manna [1], Angelino Doppiu [2], Lukas J. Gooßen [1]

[1] *Ruhr Universität Bochum, Fakultät Chemie und Biochemie, Bochum, Germany*
[2] *Umicore AG & Co. KG, Precious Metals Chemistry, Hanau-Wolfgang, Germany*

Primary anilines are of tremendous synthetic importance as building blocks for pharmaceuticals, dyes and functional polymers. For late-stage functionalization of complex molecules, the catalytic introduction of unprotected NH_2-functionalities by catalytic couplings of aryl halides with ammonia synthons is the method of choice. However, the aniline products tend to be more reactive towards arylation than ammonia, and catalytic arylation of ammonia usually yields a mixture of mono- and diarylamines.[1]

The use of pressurized gaseous ammonia is advantageous for large-scale manufacture but inconvenient for lab-scale reactions. To increase the practicality of the transformation and suppress double arylations, azides, amides, silyl amines and several other compounds have been investigated as alternative ammonia synthons but were limited by the price and availability of the reagents, the necessity of deprotection steps, or the formation of unwanted byproducts. Arguably, the most advantageous ammonia synthons are solid ammonium salts, which are utilized in the protocols by Hartwig,[2,3] Stradiotto[4] and Xue.[5]

In this work, A catalyst generated from β-methylnaphthyl (MeNAP) palladium bromide and the bulky ligand biphenyl-diadamantylphosphine (AdBrettPhos) has been found to promote the amination even of non-activated aryl chlorides with ammonium triflate within 30 min at 80 °C to the primary anilines. The efficiency of the protocol was evaluated in comparative experiments, its versatility documented by the synthesis of various primary anilines including drug-like molecules.[6]



- Broad substrate scope • Fully selective monoarylation • Up to 99% isolated yield

Figure 1: Palladium-catalyzed monoarylation of ammonium triflate with aryl chlorides

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P007

Synthesis and Investigation of copper(I)complexes with an N_3S Thioether-Ligand-System

Anna L. Scholl [1], Dr. Thomas Rotärmel [1], Prof. Dr. Siegfried Schindler [1]

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

Regarding sustainability, a long-lasting research goal has been to perform the aerobic aliphatic C-H oxidation under mild and environmentally more friendly (green) conditions.[1] In nature, some copper-containing enzymes can activate dioxygen and strong C-H bonds to perform these reactions. For example, peptidylglycine α-hydroxylating monooxygenase (PHM) that is involved in the post-translational modification of peptides.[2] The reactive species is an end-on superoxido copper complex for which a model system (with only N-donor atoms) has been developed.[3] However, the active site of PHM consists of the amino acids histidine and methionine.[4] Until now, the role of the thioether group in catalytic reactions is unclear. Therefore, different ligands with N_2S and N_3S systems have already been synthesized to mimic the active site of these enzymes, leading to different "copper-oxygen"-species.[4] Based on earlier work, a series of new N_3S and N_3 ligands (derivatives of the tripodal ligand tris(2pyridylmethyl)amine (tmpa)) were analyzed in comparison with known systems.[5]. The reactivity of the corresponding copper(I)-complexes with dioxygen was investigated by applying low-temperature UV/Vis and stopped-flow measurements between -80 °C and -140 °C. Bis(*mu*-oxo)dicopper(III) and *trans*-1,2-peroxodicopper(II)-species could thus be identified as reactive intermediates (Figure 1). The results are promising for further research in this area.

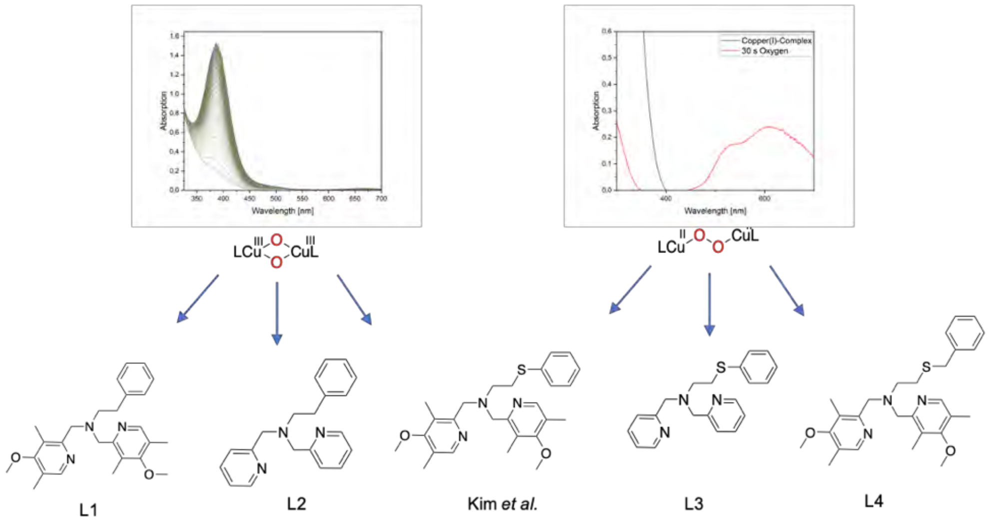

Figure 1: Synthesized ligands and formed copper-oxygen-species, with stopped-flow and UV/VIS measurements.

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P008

Inexpensive radical hydrofunctionalizations under iron catalysis

Jonas Elfert [1], Nils Lennart Frye [1], Armido Studer [1]

[1] *University of Münster, Department of Organic Chemistry, 48149 Münster, Germany*

Radical hydrofunctionalizations using metal hydrides are a mild and easy method to utilize the abundant alkene functionality to introduce new functional groups and increase the chemical value of these compounds. Compared to traditional polar hydrofunctionalizations under highly acidic conditions, they are more mild, selective and allow for introduction of a higher diversity of functional groups. Commonly, cobalt salts are utilized for the generation of the metal hydride and more rarely manganese or iron salts. Due to abundance and toxicity iron-based catalytic systems are the most desirable, but also more difficult to realize due to the multitude of available oxidation states and lower stability of catalysts. [1]

Our group recently published two papers utilizing nitroarenes as novel radical traps for hydration reactions under iron catalysis, allowing milder conditions than the commonly employed *Mukaiyama* hydration, as well as superior diasterereoselectivity. [2,3]

Building upon this, we investigated the use of other radical traps under our iron catalysis conditions. Some of which have found usage in cobalt catalysis but have not been published before for more accessible iron catalysis. We also discovered some cheaply available compounds that have not found use in hydrofunctionalizations before and allow for the introduction of new functional groups.

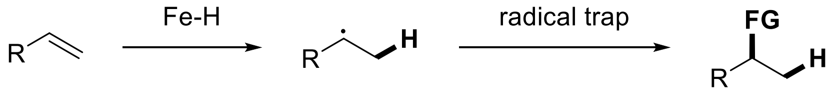

Figure 1: General scheme of a radical hydrofunctionalization.

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P009

Synthesis of phthalocyanines bearing hydroxypentyl substituted fluorene units for biological activities

Büşra Çuhadar[1], Bahareh Sajjadifard[1], Hande P. Karaoğlu[1], Ayfer Kalkan Burat[1]

[1] *Istanbul Technical University, Department of Chemistry, 34469 İstanbul, Turkey*

The chemistry of porphyrins and phthalocyanines containing novel structural subunits within or around the central macrocycle is in full development, especially for photonic applications related to cancer therapy, such as photodynamic therapy (PDT). In this regard, given the well-known oxygen photosensitizing properties of these macrocycles, the study of novel porphyrin- or phthalocyanine-based molecular assemblies that can efficiently undergo two-photon excitation while presenting significant luminescence constitutes an attractive target for researchers interested in developing novel photosensitizers for theranostic applications[1]. Porphyrins and phthalocyanines carrying fluorene groups have started to be synthesized relatively recently. Studies of fluorene-substituted phthalocyanines are more limited and few of them are relevant to their biological applications.

Fluorenes contain a rigidly planar biphenyl rings in the unit. The high reactivity of the 9,9′-position of the molecule provides substitution of various alkyl/aryl chains to fluorenes. The functionality of this position allows controlling both their solubility and other physical properties. In addition, the substitution at the 9.9' position does not have a steric effect on adjacent aromatic rings. Fluorenes have a number of advantages, such as ease of purification and characterization, well-defined structures and easily tunable luminescence and thermal properties[2-4]. Fluorene groups increase the solubility of phthalocyanines, reduce aggregation, and shift the Q bands to the red[5]. An insertion of fluorene containing moieties into the structure of phthalocyanines, has been shown as an important factor modulating their physicochemical properties, thus facilitating their potential use in biological applications. In continuation of our search for potential application of Pcs, we decided to synthesize phthalocyanines with fluorene groups as peripheral substituent's. We report herein the synthesis and characterization of peripherally tetra substituted metallo-phthalocyanines. The biological activities of synthesized phthalocyanines will be investigated.

Acknowledgements:

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P010

Tailor-made Mesoporous Metal Oxides with PEO-*b*-PHA Block Copolymers: The Role of Template Composition and Concentration

Lysander Q. Wagner [1], Frederik Breckwoldt [1], Bernd M. Smarsly [1]

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

Mesoporous metal oxides are frequently investigated as promising model materials for heterogeneous catalysts, coatings, or electric devices showing improved properties compared to their non-porous counterparts. These macroscopic properties were shown to depend on the mesopore architecture (pore size, wall thickness, and pore connectivity). Consequently, dedicated preparation protocols and deep knowledge on the templating behavior are required to (1) investigate systematically porosity-property relationships and (2) to synthesize precisely an optimized pore morphology for a desired property.

Here, we prepared a library of 15 poly(ethylene oxide)-*block*-poly(hexyl acrylate) (PEO-*b*-PHA) block copolymers of varying block lengths. While we described the general applicability of PEO-*b*-PHA as template recently,[1] we now target a quantitative study using SiO_2 as model system. According to SAXS and SEM, the PHA block is responsible for a mesopore size tuning between 20 nm (100 HA units) and 80 nm (400 HA units) independent of the PEO block. TEM-based tomography confirms a decrease in wall thickness by 50% upon increasing the ratio of template to metal oxide precursor in the sol-gel synthesis. In addition, a small increase in pore size and pore connectivity was observed enabling a fine-tuning of the pore size and connectivity by adjusting the amount of template used.

All in all, these trends provide a framework on how to tailor the mesopore morphology and enable systematic studies on *e.g.*, porous electrocatalysts to maximize stability and activity.

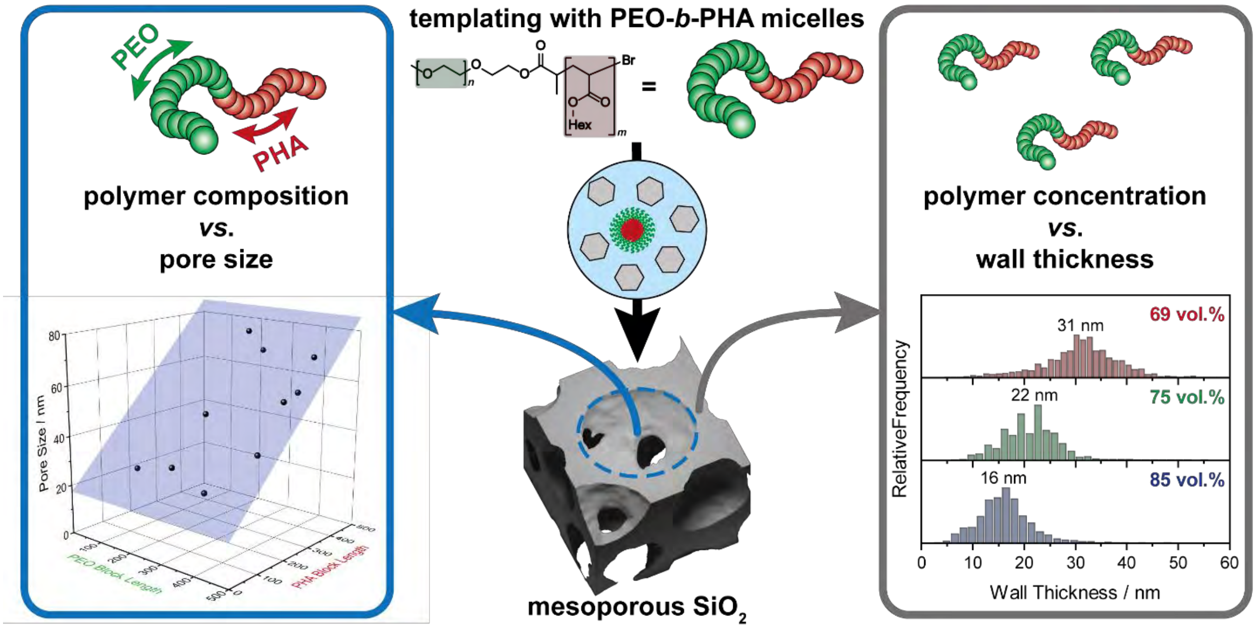

Figure 1: Tuning the mesopore morphology of metal oxides obtained by soft templating with PEO-*b*-PHA.

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P011

The novel sodium complexes of monoferrocenylspirocyclotriphosphaza-crown ethers

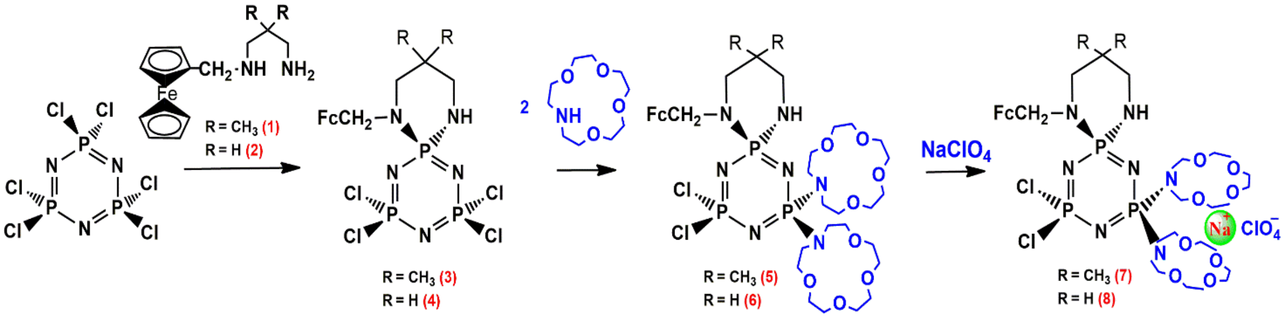
Neşe Uzunalioğlu[1], Nuran Asmafiliz[1], Zeynel Kılıç[1] and Tuncer Hökelek[2]

[1]Ankara University, Department of Chemistry, Ankara, Türkiye
[2]Hacettepe University, Department of Physics, Ankara, Türkiye

Hexachlorocyclotriphosphazene, $N_3P_3Cl_6$, (**HCCP**) is a cyclic compound consisting of three repeating PN units and has six versatile reactive Cl atoms and thermal stability. Due to these six reactive Cl atoms of $N_3P_3Cl_6$, many organic and inorganic substituted trimeric phosphazene derivatives with different properties have been prepared.[1,2]

In this study, the condensation reactions of trimer with two different diamines (**1** and **2**) yielded tetrachloromonospirocyclotriphosphazenes (**3** and **4**). These compounds and two equimolar amounts of 1-aza-15-crown-5 ether produced new monoferrocenylspirocyclotriphosphazabis(crown ether) (**5** and **6**). In addition, the complexation reactions of ditopic phosphaza-crown ethers (**5** and **6**) with $NaClO_4$ yield novel mononuclear sandwich-type sodium complexes (**7** and **8**) (Scheme 1).[3] Characterizations of phosphaza-crown ethers and complexes were performed using elemental analysis, mass spectrometry, FTIR, and ^1H, ^{13}C and ^{31}P NMR techniques. Ditopic phosphazenes (**5** and **6**) and complexes (**7** and **8**) have a stereogenic P center. They are expected to be in racemic mixtures. In addition, the crystal structure of phosphazene **5** were elucidated using X-ray crystallography. The absolute configuration of **5** was determined as R.

It is noteworthy that according to the literature survey, there is only one paper in which 1-aza-15C5 is bonded to the trimer ring.[4] Additionally, no study has been conducted on alkali and alkaline earth cation complexes of phosphaza-crown ether ligands until this study.



Scheme 1: The ferrocenylcyclotriphosphazene derivative.

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P012

Synthesis and Characterization of a Copper Dinitrogen Complex

Julie Willrett [1], Manuel Schmitt [1,2], Malte Sellin [1], Ingo Krossing [1]

[1] University of Freiburg, Institute for Inorganic and Analytical Chemistry, Freiburg, Germany

[2] University of Heidelberg, Institute for Inorganic Chemistry, Heidelberg, Germany

Since the discovery of the first transition metal dinitrogen complex in 1965,[1] research on dinitrogen complexes has flourished due to their potential applications in nitrogen fixation and activation[2] as well as their importance for fundamental chemistry.[3] Yet, no homoleptic dinitrogen complexes or dinitrogen complexes lacking strongly donating auxiliary ligands are known to date.[4]

Here we present the synthesis of the copper dinitrogen complex $[Cu\{N_2\}\{Al(OR^F)_4\}]$ ($R^F = C(CF_3)_3$) in which the formal $[Cu(N_2)]^+$ moiety is only supported by the usually weakly coordinating anion $[Al(OR^F)_4]^-$. $[Cu\{N_2\}\{Al(OR^F)_4\}]$ is prepared by reacting $Ag[Al(OR^F)_4]$ with an excess of CuI yielding insoluble AgI as a by-product. This metathesis reaction is carried out as a consecutive cascade reaction to prevent contamination of the product by Ag^+ ions (Fig. 1).

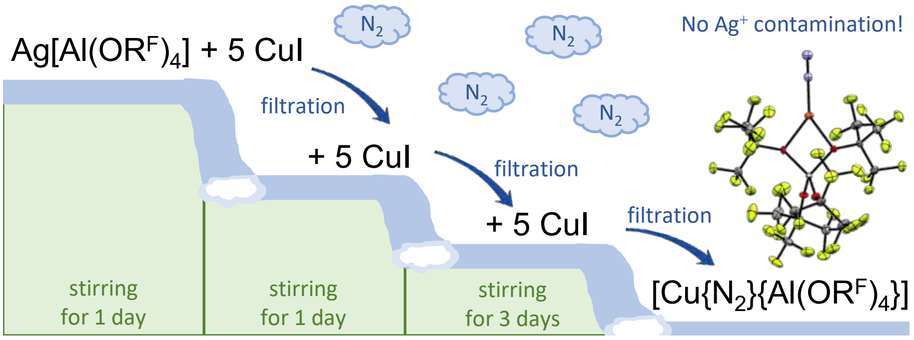

Figure 1: Cascade reaction for the synthesis of $[Cu\{N_2\}\{Al(OR^F)_4\}]$ without silver contamination.

The N_2 moiety in $[Cu\{N_2\}\{Al(OR^F)_4\}]$ is only very weakly bound which was confirmed by NMR and vibrational spectroscopy. As no strongly donating ligands are present, π backdonation into the LUMO of N_2 is reduced, resulting in an extraordinarily high N_2 stretching frequency of 2313 cm^{-1}.

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P013

Adsorptive Removal of Toxic Methylene Blue Dye Using Tea Waste-Fe_3O_4 Composite from Aqueous Solutions

Ozlem Cankurtaran[1], Meltem Guven[1], Birol Isik[1], Fatih Cakar[1]

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

Black tea is consumed in extremely high quantities in many countries and the waste parts accumulate in nature. The utilization and disposal of these wastes is very important in terms of sustainability, protection of nature, and zero waste processes.[1,2] In this study, natural, easily available, and low-cost black tea wastes were evaluated within the scope of zero waste and it was aimed to remove toxic methylene blue dye from aqueous solutions by low cost, high efficiency, and completely natural adsorption method.[3,4] Besides, a composite was prepared with Fe_3O_4 nanoparticles in order to impart magnetic properties to black tea waste and reduce the processing cost and used as an effective adsorbent for the removal of methylene blue dye from aqueous solutions. The prepared adsorbents were characterized by FTIR-ATR and SEM analysis.

For adsorption studies, firstly, the effects of physicochemical parameters such as initial solution pH, contact time, adsorbent dosage, initial concentration on the process were examined and optimum conditions were determined. After determining the optimum conditions, adsorption kinetic, and isotherm studies were carried out at different concentration values. Different isotherm models such as Langmuir, Freundlich, and Dubinin-Radushkevich (D-R) were applied to the adsorption results to determine the nature and functioning of adsorption. As a result of the experimental studies, it was found that the prepared composites fit the Langmuir isotherm model and the adsorption process takes place on monolayer and homogeneous surfaces. To investigate the adsorption kinetics and mechanism, the kinetic results were applied to *pseudo-first-order* and *pseudo-second-order* kinetic models. From the results, it was found that the adsorption process followed the *pseudo-second-order* kinetic model. Furthermore, adsorption studies were carried out at different temperatures to determine the adsorption thermodynamics.

This research has been supported by Yildiz Technical University Scientific Research Projects Coordination Department. Project Number: FBA-2023-5825.

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P014

Hydrogen transfer reactions of unsaturated model compounds with amines on carbon supported noble metals

Jacqueline Maslack [1,2], Katharina Konieczny [2], Ana Franco [2], Eszter Baráth [2]

[1] *University of Rostock, Rostock, Germany*
[2] *Leibniz-Institut für Katalyse e. V. (LIKAT), Rostock, Germany*

Transfer hydrogenations offer an easy and cheap method for the reduction of alkenes and alkynes.[1] Applying liquid hydrogen sources can avoid the use and transport of gaseous hydrogen, which poses many hazards. Furthermore, heterogenous catalysts can easily be removed from the reaction mixture and recycled.

The aim of this work was to establish an easy and fast method for the transfer hydrogenation with model substrates, containing different functional groups such as C≡C triple vs C=O double bonds (Figure 1). Our main interest was whether the supported noble metals (e.g.: Pd/C, Pt/C) proceed in a similar mode as was previously described for internal alkynes, promoting the formation of the cis alkene, and whether the reaction keeps its sequential manner.[2-3] As H-donors we used the previously successfully applied tertiary amines (e.g.: diisopropylethylamine, 1-ethylpyrrolidin), as well as secondary amines (e.g.: indoline) to get insight into the potential H-donation ability of such molecules and compare their effectiveness with their tertiary counterparts. Secondary amines are also considered as good H-donors. However, due to the presents of the free (N)H group, they tend to initiate undesired side reactions depending on the actual reaction conditions. During our study, we characterized the always pre-reduced catalysts, recorded kinetics in the initial regime of the reaction and tried to link the observed conversion/selectivity pattern to the catalytic activity of the metals.

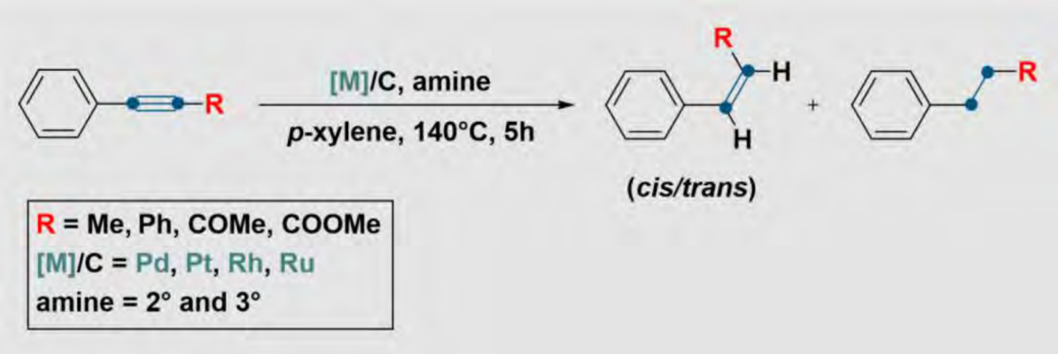

Figure 1: Hydrogen transfer reactions with substituted alkynes.

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P015

Molecular Dynamics Simulations as a tool to investigate the impact of imidazole-based cholesterol in lipid bilayers

Clara Rickhoff [1], Azadeh Alavizargar [1], Andreas Heuer [1]

[1] *University of Münster, Institut für Physikalische Chemie, Münster, Germany*

For the investigation of plasma membranes in mammalian cells cholesterol is of special interest, as this molecule has a significant impact on their structure and fluidity. Thus, experiments visualizing cholesterol are an important tool to deepen the understanding of cellular membranes. These experiments are facing the difficulty of tracking cholesterol, as this molecule is not fluorescent. In order to overcome this problem imidazole-based cholesterols were developed, which allow to add functionalities to a cholesterol analog without changing the backbone which is embedded in the membrane.[1]

In our work we conducted Molecular Dynamics simulations of a non-charged imidazole-based cholesterol, which was previously synthesized in the Glorius group (University of Münster). With these simulations we investigated the impact on the structure of lipid bilayers as well as its impact on the stability of lipid rafts, when replacing cholesterol by this novel molecule. The analysis of the order parameter, the tilt angle and the position of the different cholesterols within a bilayer allows a more precise assessment of how accurate this analog mimics cholesterol also compared to the positively charged imidazolium-based analog.

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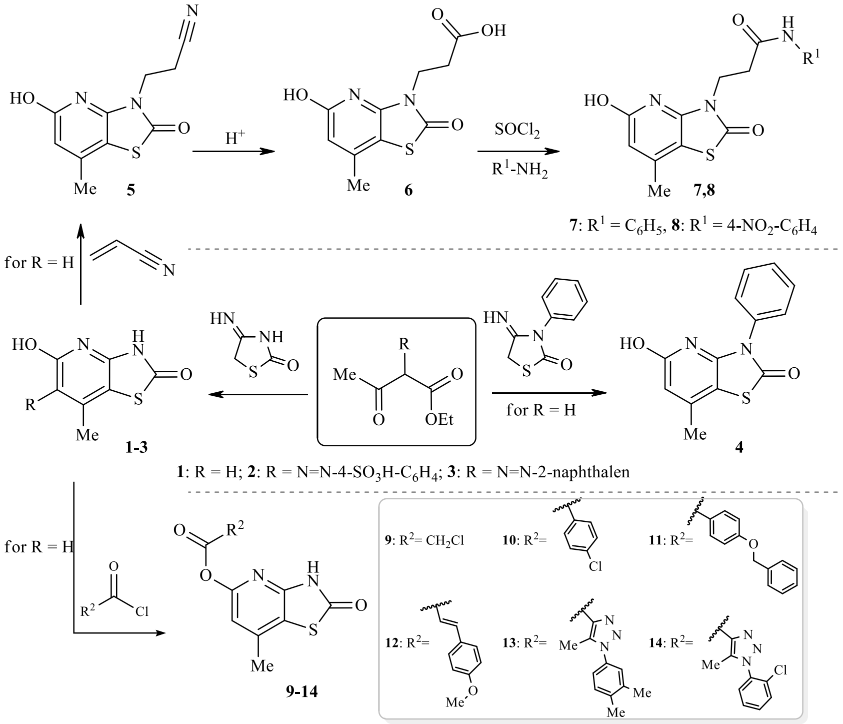
P016

Synthesis, molecular docking and anti-inflammatory activity of some thiazolo[4,5-*b*]pyridines

Anastasia T. Vachko [1], Taras I. Chaban [1], Olga Ya. Shyyka [2], Olena. V. Klenina [1], Iryna V. Drapak [1], Ihor G. Chaban[1], Vasyl S. Matiychuk [2]

[1] Danylo Halytsky Lviv National Medical University, Lviv, Ukraine
[2] Ivan Franko National University of Lviv, Lviv, Ukraine

Thiazolopyridines, as purine bioisosteres, are an important type of heterocyclic systems. Their intensive study is driven by both a considerable range of their pharmacological activity and synthetic capabilities for functionalization of derivatives at different positions. Published scientific data have confirmed that annelated thiazolopyridines have a various biological activity. They include substances with antioxidant, antimicrobial, anti-inflammatory, and antifungal activities which are agonists of H3-histamine receptors, and substances with high inhibitory activity against epidermal growth factor receptors and against a number of other enzymes.[1] Continuing systematic study of fused bicyclic systems as potential drug candidates we represented synthesis, anti-inflammatory activity evaluation of some thiazolo[4,5-b]pyridin-2-ones. Fused thiazolo[4,5-*b*]pyridin-2-ones were synthesized and modified at the N^3, C^5 and C^6 positions of the main core in order to obtain the compounds with a satisfactory pharmacological profile. The synthesized compounds were preselected *via* molecular docking for further testing of their anti-inflammatory activity *in vitro*. Evaluation of novel compounds over the carageenin induced rat paw edema revealed strong anti-inflammatory action of some compounds including (thiazolo[4,5-*b*]pyridin-3(2H)-yl) propanenitrile (**5**) and thiazolo[4,5-*b*]pyridin-3(2H)-yl) propanoic acid (**6**) even exceeding the standard – Ibuprofen.



In summary, we presented an efficient synthetic approaches to a number of thiazolo[4,5-*b*]pyridin-2-one derivatives for their anti-inflammatory activity evaluation. The obtained results of the performed biological activity evaluation suggested the core fused heterocycle as a promising scaffold in anti-inflammatory drug development.

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Advancements in 3D Bioprinting: Bridging Technology and Tissue Engineering for Enhanced Bone Scaffold Fabrication

Paulina Sobierajska [1], Katarzyna Wiglusz [2] and Rafal J. Wiglusz [1,3]

[1] 1Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okolna 2, 50-422 Wroclaw, Poland
[2] Faculty of Pharmacy, Medical University of Wroclaw, Borowska 211A, 50566 Wroclaw, Poland, p.sobierajska@intibs.pl
[3] Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, Faculty of Chemistry, Silesian University of Technology, Krzywoustego 4, 44100 Gliwice, Poland

Over the past two decades, the 3D bioprinting has undergone significant technological advancements. It was initially employed for crafting small-scale models and prototypes, and has evolved into a versatile technology with applications spanning various fields including bone tissue engineering[1]. The primary challenge in bioprinting systems lies in bioink materials. The bioinks must meet specific viscosity requirements for the chosen printing method. For extrusion-based bioprinting, the bioink needs to exhibit shear thinning and rapid shear recovery, facilitating smooth extrusion and maintaining the intended shape upon deposition. This enables the creation of large, high-resolution structures[2]. In addition to printing demands, the resulting structure should have suitable mechanical properties for sustained shape fidelity and easy handling. The bioink should support long-term cell culture.

3D printed scaffolds made solely of pure nanocrystalline hydroxyapatite (nHAp) exhibit poorer mechanical properties when compared to those composed of a combination of nHAp and synthetic polymers. Pluronic has been employed in combination with nHAp to fabricate nHAp-based structures, aiming to improve their structural manipulability, flexibility, and versatile mechanical performance[3]. The production of 3D-printed scaffolds (Fig. 1) could significantly gain from a manufacturing method that allows meticulous fabrication to replicate the natural bone's morphology. This includes achieving controlled interconnected porosity and specific pore sizes, promoting the infiltration of new bone, and facilitating the gradual degradation of the scaffold.

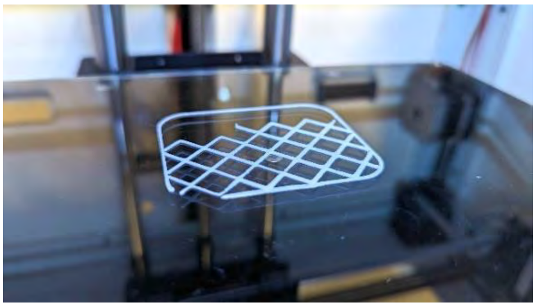

Figure 1: 3D printing of nHAp/Pluronic-based bone scaffold.

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P018

JCF Team Sustainability - Joined voices for more sustainability.

Hannah Kortman [1], Felix Katzenburger [2], Alena Neudert [3]

[1] *Max-Planck-Institut für Kolloid- und Grenzflächenforschung, 14476 Potsdam, Germany*
[2] *Westfälische Wilhelms-Universität Münster, Organisch-Chemisches Institut, 48149 Münster, Germany*
[3] *Julius-Maximilians-Universität Würzburg, Institut für Funktionsmaterialien, 97070 Würzburg, Germany*

Sustainability is a timely topic of immense societal relevance in which chemistry has a key role to play. JCF's Sustainability Team is built around the central question: "How can we as young chemists contribute to a sustainable future and inspire others to take action?" In the team, we discuss ideas and initiate projects to raise awareness and promote sustainability through practical approaches. Previous projects include a sustainability guide, the design of sustainable JCF giveaways, a survey to assess the appropriateness of sustainability in education, and a white paper that presents young chemists' views on this topic in the context of the UN Sustainable Development Goals (SDGs).[1,2]

Figure 1: Logo of the JCF Team Sustainability.

Currently we are working on bringing sustainable chemistry to high schools, establishing connections between young chemist, academia and industry, and communicating more sustainable lab practices. With these initiatives, we want to promote sustainability on different levels, by making the work of the JCF itself more sustainable, fostering the ambitions and initiative of young chemists on a national and international stage and giving young chemists a voice in shaping a more sustainable future. We are always looking for new creative ideas and welcome motivated team members who would like to participate in their realisation.[3]

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[3] JCF Team Sustainability Homepage https://jcf.io/teams/nachhaltigkeit (accessed 09.01.2024).

P019

Oxidation of Acetol – An Approach using Green Chemistry Principles

Isabell Prediger [1], Carmen Albers [2], Juliane Witzorke [2], Sebastian Schwarze [2],
Nora Kulak [1,2]

[1] University of Potsdam, Institute of Chemistry, Potsdam, Germany
[2] Otto-von-Guericke University Magdeburg, Institute of Chemistry, Magdeburg, Germany

Oxidation reactions usually are connected to loads of dangerous conditions and waste. For example, Cr(VI) chemistry is widespread as it is well known for its oxidative properties, which can be controlled through the variation of reaction conditions and additives, however, it is highly cancerogenic.[1] Regarding the principles of green chemistry that contain a zero waste policy as well as the usage of mostly harmless solvents and chemicals, we tried an environmentally compatible approach using earth-abundant metals. Their ability of one-electron-transfers in combination with an oxidant like H_2O_2 or *tert*-butylhydroperoxide (TBHP), show first positive results in catalysing an oxidation reaction, here using simple salts of iron and copper.[2, 3]

For this purpose, we chose the α-hydroxy ketone acetol, as it is the simplest example for this structure type. The goal was the analysis of possible products as well as the selectivity. In general, five main products could be identified via HPLC (*see Figure*).

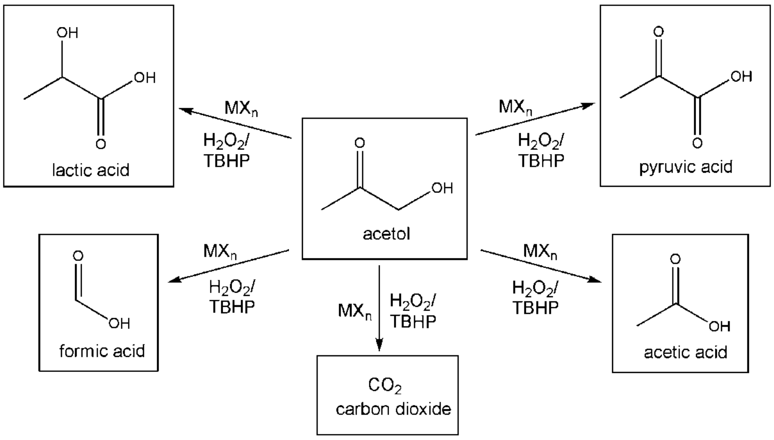

Figure 1: Possible reaction paths for the catalytic oxidation of acetol.

The variation of the catalyst, their concentration as well as the choice of the oxidant show a correlation between the degree of oxidation and the conversion rate. E.g. the iron salt Fe(**III**) chloride shows 100% conversion rate. The main products are formic and acetic acid as well as presumably CO_2. In contrast, some copper salts such as Cu(II) chloride lead to a mixed product profile (all products presented in Fig. 1), but only yield up to 35% conversion. The omission of either the catalyst or the oxidant results in an only marginally observable reaction. Hence, the oxidation power is decisive for the conversion rate. Thus, the selectivity needs to be optimized in further experiments by varying and broadening the conditions.

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P020

Synthesis, Characterization and Exploring of Sono-Photochemical Activities of New Halogen-Containing Zinc Phthalocyanines

Sena Nur Alegöz[1], Ali Erdoğmuş[1]

[1] *Yıldız Technical University, Institute of Science and Technology, Istanbul, Turkey*

Photodynamic therapy (PDT), sonodynamic therapy (SDT) and sono-photodynamic therapy (SPDT), the combination of these two methods, are quite remarkable methods in the treatment of cancer, one of the most important health problems of our age. [1] Photodynamic therapy is based on the principle of destroying tumor cells as a result of the production of reactive oxygen species (ROS), especially singlet oxygen, by the photosensitizer stimulated by light. [2] In sonodynamic therapy, ultrasound replaces light and produces sonosensitizer singlet oxygen. [3] Novel studies have shown that sono-photodynamic therapy, performed with the synergetic effect of light and sound, produces singlet oxygen with higher efficiency and causes cell death more effectively. [4] The functionality of PDT, SDT and SPDT depends on the photo-sonosensitizer used in the therapy. Zinc phthalocyanines (ZnPcs) are used as second-generation photosensitizers in PDT, thanks to their superior properties. [5]

In this study, zinc phthalocyanines tetra-substituted with 4-Chlorothiophenol and 4-Bromothiophenol moieties at peripheral positions were synthesized and characterized by FT-IR, mass spectroscopy and electronic spectroscopy. And then their sonochemical, photochemical and sono-photochemical abilities were measured and compared. Comparative measurements showed that differences were observed in the efficiencies obtained by halogen exchange and the sonochemical method showed a more effective therapeutic effect than the photochemical method. It is also shown that the synthesized compounds can be used as promising SPDT agents in future in vivo and in vitro studies.

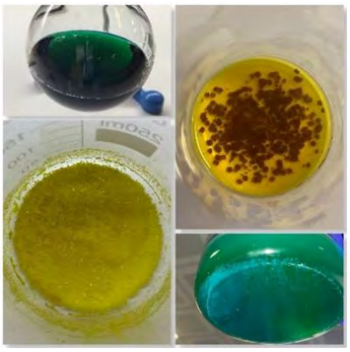

Figure 1: 4-Chlorothiophenol and 4-Bromothiophenol substituted Phthalocyanine Derivatives.

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P021

Investigation of Surface Properties of Hyaluronic Acid by Inverse Gas Chromatography

Sadan Yurtcu Celik[1], Ayse Erdogan Cakar[1], Ozlem Yazici[1]

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

Inverse gas chromatography (IGC) is a specialized technique used to characterize the surface and bulk properties of materials. Unlike traditional gas chromatography, where a volatile sample is separated based on its interaction with a stationary liquid phase, IGC reverses the roles by using a non-volatile probe gas to interact with the surface of the sample.[1,2] IGC is particularly used for studying the surface properties of materials, including polymers, biopolymers, liquid crystals, pharmaceuticals, composites, etc. Biopolymers play a crucial role in various industries, including health, food, and cosmetics, owing to their biocompatibility, cost-effectiveness, abundance in nature, and sustainable characteristics.[3] Consequently, the surface properties of biopolymers hold significant importance in facilitating the industrial applications of these materials. Among biopolymers, hyaluronic acid (HA) is a versatile and essential component in the human body, contributing to joint health, skin hydration, and various medical and cosmetic applications. Its ability to retain water and maintain tissue integrity makes it a valuable substance in the field of healthcare and beauty.[4]

In this study, HA surface properties were investigated using the IGC method. The IGC studies were conducted over a temperature range spanning from 303.2 to 328.2 K. Utilizing the net retention times within these temperature intervals, we determined both the dispersive surface energy and the acidic-basic nature of the surface of HA through the use of polar and non-polar probes. Additionally, specific adsorption free energy and specific adsorption enthalpy values, indicative of acid-base surface interactions, were calculated. Through correlation with the donor and acceptor numbers of the probes, we derived insights into the acidic and basic surface properties of the HA.

This research has been supported by Yildiz Technical University Scientific Research Projects Coordination Department. Project Number: FBA-2023-5838

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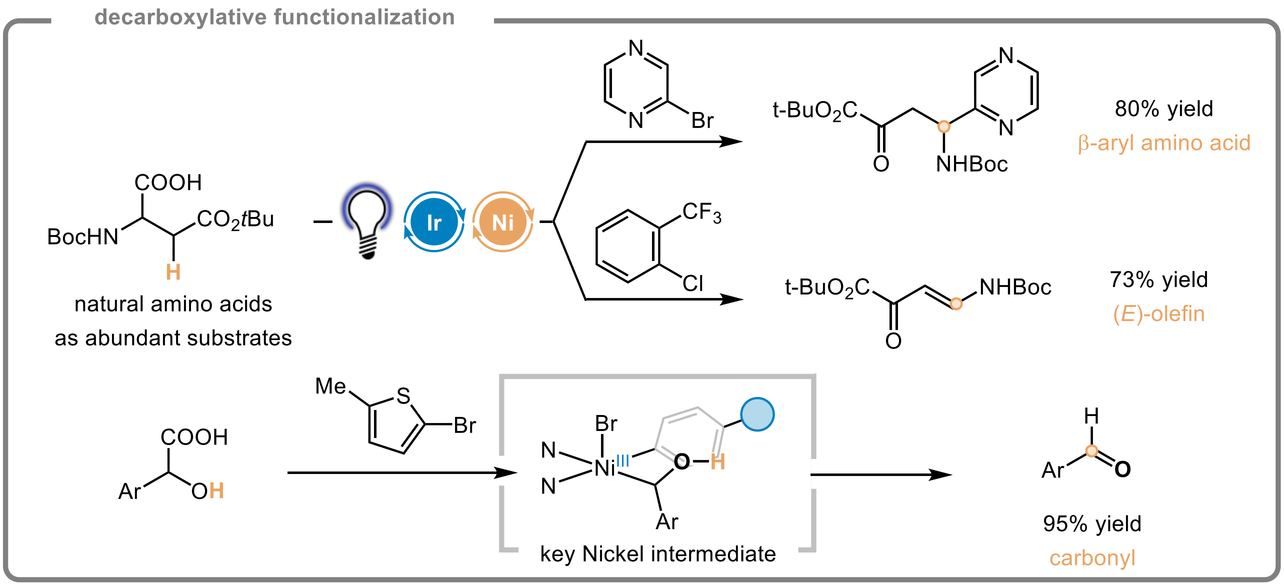
P022

Electronic Modulation facilitates Decarboxylative Elimination and Arylation

N. Wei, B. Stouwie, A. Garcia-Castillo, S. B. Beil[1]

[1] *University of Groningen, Stratingh Institute for Chemistry, Groningen, NL*

Metallaphotoredox catalysis has greatly expanded the capacities of transition metal catalysis. Especially, Nickel-photoredox catalysis has been proved to be an effective strategy to enable elusive cross-coupling from abundant, native functional groups.[1,2] Our research aim is to utilize natural amino acids as a radial precursors to distinguish the selectivity of elimination and arylation under identical conditions.[3] The selectivity is achieved by modulating the oxidation state of Ni and the electronic properties of auxiliary additives. The selectivity is enhanced by altering the electronic properties of oxidant, *e.g.*, bromobenzene. This alternation influences the rate of arylation vs. elimination *via* a resonance effect.[4] Specifically, the higher electron-donating ability of bromobenzene suggested that the elimination is pronounced. Oppositely, the electron-withdrawing substitutions on the bromobenzene dominated the arylation transformation. Besides, the ortho-, meta-, and para-substitution effect on aryl halides in relation to elimination and arylation selectivity will be discussed. Other effects, such as solvent and bases are also important with regards to the selectivity. This methodology achieves the formation of β-aryl amino acids, olefins, and carbonyl compounds in moderate to excellent yields.



Scheme 1: General scheme of the selectivity modulation between arylation and elimination in nickel photoredox catalysis.

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P023

Stability improvement of peptide drug candidates targeting the Complement Cascade

Tom Götze [1], Bekas Alo[1], Stephanie Vogt[2], Carla Johanna Sommer-Plüss[2], Daniel Ricklin[2], Christina Lamers[1]

[1] Institute for Drug Discovery, Medical Faculty, Leipzig University
[2] Molecular Pharmacy, Department of Pharmaceutical Sciences, University of Basel, Switzerland

The Complement Cascade, an integral component of the innate immune system, consisting of a sophisticated interplay involving more than 30 plasma proteins. Despite its complexity, susceptibility to misregulation can have profound consequences for the organism.

Peptides have emerged as compelling candidates for therapeutic intervention, exhibiting the potential to target proteins lacking distinct binding pockets necessary for interaction with conventional small organic molecules. Capitalizing on their automatable synthesis, non-toxic metabolites, and exceptional target specificity, peptide therapeutics epitomize a strategic convergence between small molecules and large biologicals.[1]

However, a critical limitation of peptide therapeutics resides in their intrinsic challenge of low bioavailability, given their rapid metabolic degradation by endogenous proteases.

This study aims to establish a robust analytical method for monitoring the stability of peptide drug candidates within blood plasma. The compounds of interest, derived from a phage display screening targeting the ligand-binding α_{M}I domain of Complement Receptor 3 (CR3), exhibit intriguing behaviour, selectively inhibiting receptor binding to various disease relevant endogenous ligands.[2]

Our findings reveal promising half-lives in the current stage of drug development for the investigated peptide. Ongoing optimizing efforts focus on implementing stability enhancement strategies, crucial for advancing the development of cutting-edge Complement Modulators. This research is contributing to offering novel therapeutic avenues for addressing immune-related disorders.

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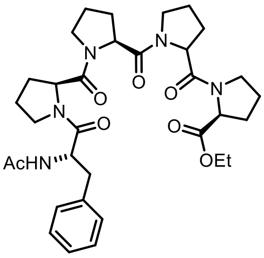
P024

Designed EVH1 inhibitors derived from synthetic diproline mimetics (ProMs) rigidified in a PPII helix conformation

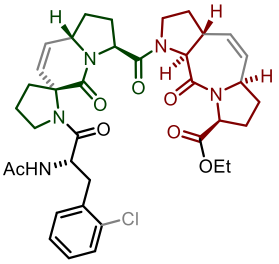
F. Blüm [1], M. Barone [2], M. Müller [2,3], D. Albat [1,3], S. Chiha [1,3], R. Kühne [2], H.-G. Schmalz [1]

[1] Department of Chemistry, Department of Chemistry, Köln, Germany
[2] Leibniz-Institut für Molekulare Pharmakologie (FmP), Berlin, Germany
[3] PROSION GmbH, Köln, Germany

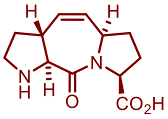
We combined computational modeling, X-ray crystallography, organic synthesis and biological investigations to develop small-molecule inhibitors for the Ena/VASP EVH1 domain, which is involved in the migration and chemotaxis (metastasis) of invasive cancer cells.[1] Using synthetic diproline mimetics such as **ProM**-1,[2a] **ProM-2**,[2b] **ProM-13**[2c] and **ProM-15**[2d] we succeeded to reduce the wild-type oligopeptide sequence **WT1** to an equivalent of the pentapeptidic proline rich core sequence **WT2**, which itself only shows weak binding. By freezing pairs of prolines in a PPII helix conformation (by formal introduction of a vinylidene bridge) in combination with the introduction of a chlorine atom to the phenylalanine residue, the first nanomolar EVH1 inhibitors (**L1**-**L3**) were obtained.[1]



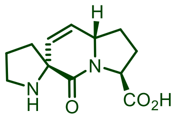
Ac-**FPPPP**-OEt



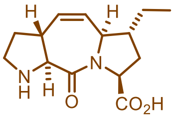
Ac-**[2-Cl-F][ProM-2][ProM-1]**-OEt



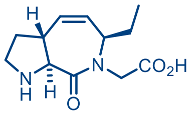
H**[ProM-1]**OH



H**[ProM-2]**OH



H**[ProM-13]**OH



H**[ProM-15]**OH

Ligand	Ligand composition	K_d [µM]	ΔG [KJ mol^{-1}]
WT1	Ac-SFE-**FPPPP**-TEDEL-NH_2	13.0 ± 0.6	-27.9 ± 0.1
WT2	Ac-**FPPPP**-OEt	153 ± 8	-21.9 ± 0.1
L1	Ac-**[2-Cl-F][ProM-2][ProM-1]**-OEt	4.1 ± 0.3	-30.8 ± 0.2
L2	Ac-**[2-Cl-F][ProM-2][ProM-15]**-OMe	0.47 ± 0.03	-36.1 ± 0.1
L3	Ac-**[2-Cl-F][ProM-2][ProM-13]**-OEt	0.12 ± 0.01	-39.5 ± 0.3

Besides exhibiting strong affinity, the optimized inhibitors were shown to bind to the EVH1 domain in the canonical fashion. While *in vitro* cell-migration experiments which proved the inhibition of chemotaxis, the extravasation of MDA-MB-231 cancer cells was demonstrated *in vivo* using transgenic zebrafish embryos.[1b] Notably, the compounds showed high selectivity towards EVH1 in comparison to other proline-rich motif-recognizing (off-target) protein domains (Fyn SH3, Profilin, Yap1 WW1) as revealed by $^{1}H^{15}N$ HSQC NMR experiments.

References:

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P025

Investigating vibrationally assisted Chiral Induced Spin Selectivity

Thibaut Lacroix [1], James Lim [1], Susana F. Huelga [1], Martin B. Plenio [1]

[1] Ulm University, Institute of Theoretical Physics and IQST, Ulm, Germany

The Chiral Induced Spin Selectivity (CISS) is an phenomenon where the chirality of an organic molecule induces a spin-dependence of the charge transport, resulting in the spinpolarization of electrons transmitted through the molecule.

This robust effect has been observed in several experiments involving both photoelectrons being transmitted through mono-layers of helical molecules (such as DNA), as well as bound electrons transmitted through chiral molecules placed in between two electrodes.

This effect has interesting consequences for the development of spintronic nanodevices, but also opens fascinating lines of investigation regarding the origin of homo-chirality in living organisms, and could play a role in several biological processes involving charge transfer (e.g. respiration). Furthermore, recent interest has sparked about the interplay between electron spin and enantioselectivity in chiral molecules.

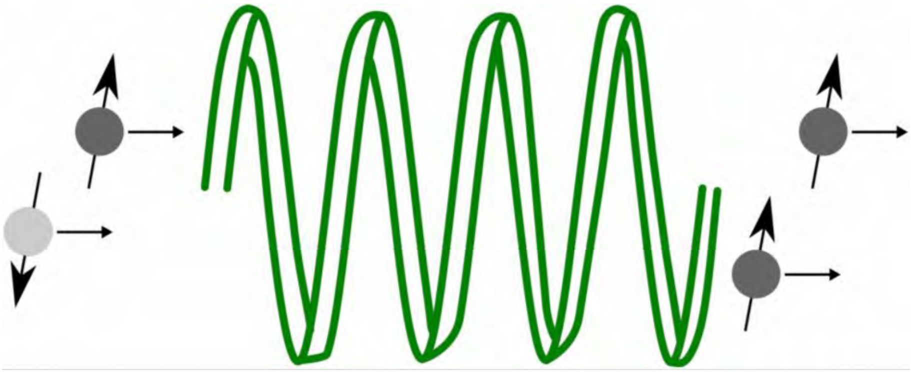

Figure 1: Electron transmitted through chiral organic molecules are spin-polarized. There is no consensus on the microscopic origin of this effect.

Even though the spin-orbit coupling (SOC) originating from the chirality of the molecules is regarded as a central part of the explanation of the CISS effect, to this day there is no consensus opinion on its microscopic origin.

In a previous work[1] it has been demonstrated, within a single electron model, that the non-equilibrium dynamics of delocalized phonon modes in chiral molecules induce fluctuations in the SOC experienced by a propagating electron. These fluctuations lead to biased spin-flips that constitute a mechanism for the CISS effect.

Following this line we investigate, using the framework of the theory of open quantum systems, the role of localized and delocalized molecular vibrations in the spin polarization of electrons transmitted through chiral molecules.

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P026

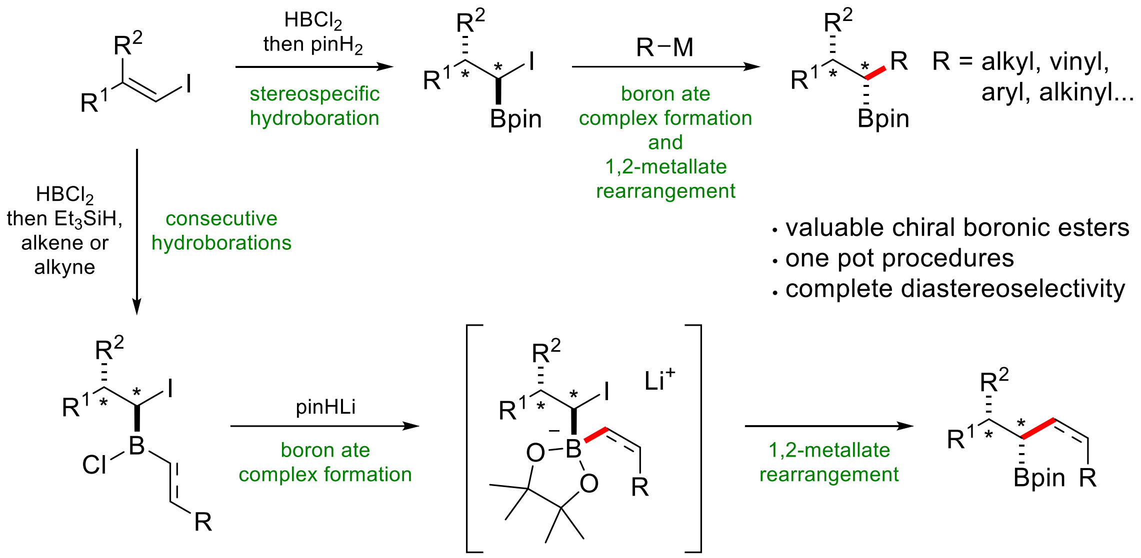
Borylative Transition Metal-Free Couplings of Vinyl Iodides with Various Nucleophiles, Alkenes or Alkynes

Gesa Seidler [1,#], Max Schwenzer [1,#], Florian Clausen [1], Constantin G. Daniliuc [1], and Armido Studer [1].

[1] Universität Münster, Organisch-Chemisches Institut, 48149 Münster, Germany

[#] M. S. and G. S. contributed equally to this work.

Boronic esters are highly valuable compounds in organic synthesis and related fields.[1] Herein, stereoselective borylative coupling reactions of vinyl iodides with various compound classes are disclosed. A stereospecific hydroboration (with $HBCl_2$) allows for the catalyst-free formation of α-iodo boron compounds which are valuable intermediates in cascades including a stereoselective 1,2-metallate rearrangement (Scheme 1).



Scheme 1: Stereospecific borylative couplings of vinyl iodides with organometallics (top) and alkenes or alkynes (bottom) via a cascade of hydroboration(s) and 1,2-metallate rearrangement.

Differently hybridized carbanions can be used to induce the rearrangement when the hydroboration is followed by trapping with a diol forming an α-iodo boronic ester. Alternatively, a second hydroboration may be appended before trapping with a diolate to trigger the rearrangement, enabling the cross coupling with alkenes or alkynes.The developed methods allow for the completely diastereoselective construction of complex alkyl boronic esters from simple starting materials and can be conducted as one pot processes.

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P027

Synthesis and Characterization of a Novel Triazole- and Piperazine-Derivative Schiff Base Compound

Perihan Kızılkaya, Nesrin Beynek

Trakya University, Department of Chemistry, Edirne, Türkiye

It is obvious that the pharmaceutical industry must constantly develop and the need to synthesize molecules that can be new drug candidates. As it is known, the most preferred method in the treatment of many diseases is the use of biological active agents. It is observed that many approved drugs and drug candidate molecules in clinical studies contain nitrogen-containing heterocyclic structures. At the same time, the biological properties of these structures appear to be pharmacologically applicable, and the importance of developing various synthesis designs to investigate their biological effects has been demonstrated by numerous studies [1,2]. Triazole derivative compounds have been shown to have clinical importance due to their biological properties, and it has been emphasized that there is a trend towards the use of these molecules in drug candidate molecule designs [3]. Piperazine heterocyclic ring is found in drugs used in the treatment of many diseases and appears to be indispensable structures in the development of new therapeutic agents with its wide range of pharmacological properties [4]. In this study, it has been aimed to further increase the biological activity by using the Schiff base reaction to bring these units together (Figure 1). In order to obtain the new Schiff base compound (**L**), firstly, the aldehyde compound containing the triazole group formed by the click reaction was synthesized, and then the condensation reaction of this aldehyde with the amine group containing the piperazine derivative was carried out and all compounds resulting from the reaction were purified. On the other hand, biological activity studies of this compound will be investigated.

Acknowledgement: We would like to thank TUBITAK (Project No:123Z163) and TUBAP (Project No:2023/180) for financial support for this work.

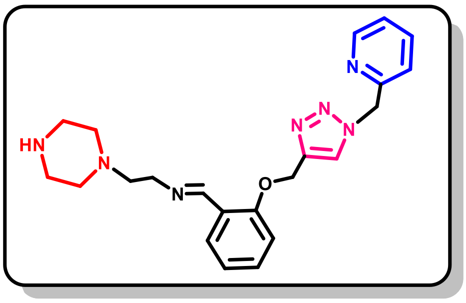

Figure 1: A new Triazole- and Piperazine- Derivative Schiff Base Compound (**L**).

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P028

Stabilized analogues of Z-RNA and their interaction with Z-nucleic acid binding immune response proteins

Finn Dicke [1], Stephanie Kath-Schorr[1]

[1] *University of Cologne, Department of Chemistry, Cologne, Germany*

While double-stranded nucleic acids usually form right-handed helices under physiological conditions, they can also exist as left-handed double helices termed Z-DNA/RNA after the zigzag-structure of the phosphate backbone. Z-helix formation mostly occurs in regions with alternating (G-C)-repeats with G being in *syn*- and C in *anti*-conformation.[1] Although Z-helices are rather unfavoured and require high-salt concentrations for stabilization,[2] Z-nucleic acids play an important role as they are recognized by Zα protein domains found in immune-signalling proteins adenosine deaminase acting on RNA (ADAR1) and Z-D/RNA-binding protein 1 (ZBP1).[3] These proteins are known to localize in cytoplasmic stress granules under conditions of cellular stress conditions.[4]

To investigate the role of Z-nucleic acids in immunoregulatory pathways and specifically their interaction with the Zα domain, modified nucleic acids that form stable Z-helices under physiological conditions are needed. For that, C8-substituted guanosine derivatives which prefer *syn*-conformation[5] are prepared and used in solid-phase synthesis of oligonucleotides. Structure characterization of the synthetic Z-RNA will be performed by CD and NMR spectroscopy and binding to the Zα domain will be investigated. In a further step, fluorescent Z-RNA duplex analogues will be employed to track Zα domain proteins in cells by confocal fluorescence microscopy under cellular stress conditions.

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P029

Theoretical studies investigating the mechanism of methanol formation over a Cu/ZnO based catalyst

David A. Jurado A.[1], Michael D. Higham[2], C. Richard A. Catlow[2], Ingo Krossing[1]

[1] Universität Freiburg, Institut für Anorg. & Analyt. Chemie 79104 Freiburg, Germany
[2] University College London, Dept of Chemistry, WC1H 0AJ London, UK

Cu/ZnO-based catalysts have been used to synthesize MeOH from syngas ($CO/CO_2/H_2$) for almost 60 years. MeOH production is a major industrial process, reaching 311 million tons per year in 2030 and growing. However, the mechanism of MeOH formation via CO_2 hydrogenation remains under discussion. Key areas of debate are the role of O defects/ vacancies on the ZnO surface, Cu-Zn synergism at the interface, the formation of Cu/Zn alloys, the role of ZnO (i.e. SMSI), etc.[1,2,3]

Methodology: All periodic DFT calculations were performed using the software *VASP*, using the PAW approximation for the core-valence interactions and PBE_{Sol} as exchange-correlation functional. The system consists of 230 atoms in a 3D periodic slab model[4].

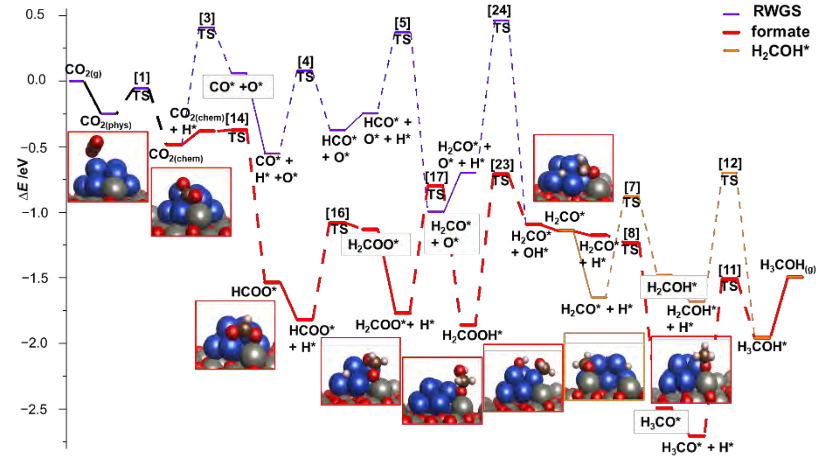

Figure 1: Preferred MeOH pathway for the Cu/ZnO system following the formate and RWGS pathway. NB: Gas species were omitted from the reaction equation to provide a clearer view. For the images red is reserved to O atoms, brown for C, blue for Cu, grey for Zn and white for H. Transition states (TS) are denoted with dashed lines.

Results and discussion: All relevant intermediates to the MeOH synthesis were investigated on a realistic model catalyst surface. We analysed different surface sites, stabilities, activation of species on the surface and activation barriers for relevant elementary processes. In this, we emphasize on the role of CO_2 activation on a Schottky barrier, formate stability and active site regeneration. Our analysis explains that MeOH would be form following the formate path on the interfacial Cu/Zn site of a Cu/ZnO catalyst.

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Synthesis and characterization of novel tetra alkynyl substituted metallo-phthalocyanines

Bahareh Sajjadifard[1], B şra Çuhadar[1], Hande P. Karaoğlu[1], Ayfer Kalkan Burat[1]

[1] *Istanbul Technical University, Department of Chemistry, 34469 İstanbul, Turkey*

In recent times, the spotlight has increasingly turned towards the multifaceted applications of phthalocyanines (Pcs), intricate aromatic macrocyclic compounds characterized by four isoindoline groups and an 18-π electron system[1]. This attention is notably directed towards their potential role in advancing photodynamic therapy (PDT) for cancer treatment. Their adeptness in absorbing tissue-penetrating red light and proficiently generating singlet oxygen positions them as promising contenders in PDT studies. The incorporation of anionic and cationic groups, such as carboxylate, sulfonate, or quaternized ammonium groups, enhances their water solubility, a crucial aspect for efficient administration into body tissues. The versatile properties of these synthetic macrocycles enable new advances at the intersection of molecular science and medical applications.

In the field of organic chemistry, fluorene is an interesting polycyclic aromatic hydrocarbon with a distinctive molecular structure. Composed of two benzene rings fused together, fluorene stands out for its notable stability and intriguing electronic properties. Fluorene derivatives have found applications in various scientific fields, including materials science and optoelectronics, due to their ability to serve as building blocks for semiconductors and organic light-emitting diodes (OLEDs)[2]. They are also interesting as luminescent materials, as the conjugated system in fluorine contributes to their photophysical properties. Besides its role in materials science, fluorene derivatives have also shown potential in medicinal chemistry and exhibited promising biological activities[3]. Since the number of studies on biological applications of fluorene derivatives is still limited, in this study the synthesis and characterization of metallo-phthalocyanines bearing alkynyl-fluorene groups in their peripheral positions are given.

Acknowledgements:

This work was supported by TUBITAK (Project Number: 122Z467).

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P031

Synthesis and spectroscopic properties of novel heteroleptic zinc(II) aza-dipyrromethene complexes bearing 2-(morpholin-4-yl)ethoxy groups

Milena Kasprzak [1], Michal Kryjewski [1]

[1] *Poznan University of Medical Sciences, Chair and Department of Inorganic and Analytical Chemistry, Rokietnicka 3, 60-806 Poznan, Poland*

Aza-dipyrromethenes (ADPMs) are a class of synthetic molecules with strong absorption in the visible light and near-IR region.[1] Due to their optical properties, ADPM derivatives are considered as photosensitizers for photodynamic therapy. ADPMs are ligands that can form complexes with BF_2^+ (aza-BODIPYs), or with a wide range of metal cations, especially of d-block transition metals (e.g. Zn, Co, Ni, Co, Rh, Pt, Pd). Metallic complexes are obtained by direct reaction of metal salt and ADPM ligands bearing specific substituents.[1,2]

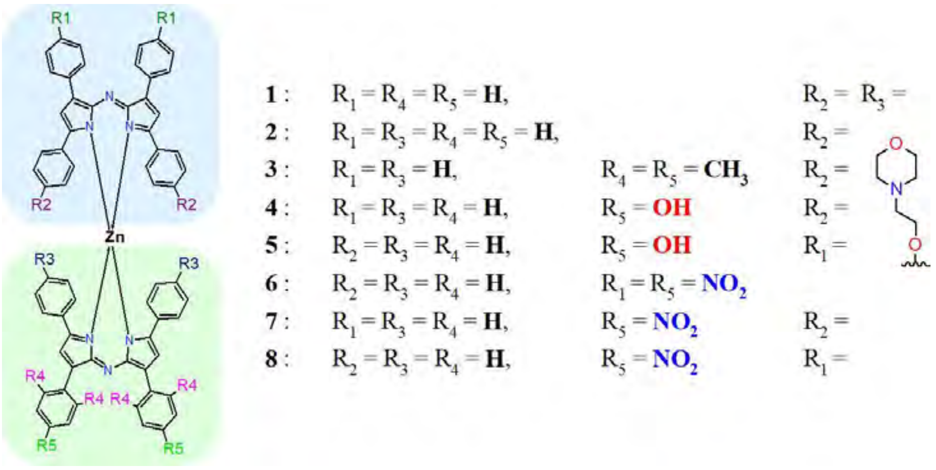

Figure 1: All synthesized zinc(II) aza-dipyrromethene complexes

The aim of the study was to synthesize and investigate optical properties of novel heteroleptic zinc(II) aza-dipyrromethene complexes bearing different substituents – hydroxyl, nitro, methyl and 2-(morpholin-4-yl)ethoxy groups on the phenyl rings. Each mixed complexation reaction of two different ligands with zinc(II) acetate resulted in the formation of three different compounds – one heteroleptic (ZnAB) and two homoleptic complexes (ZnA_2, ZnB_2), which were separated using chromatographic techniques. Six novel heteroleptic and two novel homoleptic complexes were synthesized and characterized. Molecular structures were investigated using NMR analyses and mass spectrometry (MS/ESI). UV-VIS studies were conducted in four solvents: toluene, chloroform, tetrahydrofuran (THF) and N,N-dimethylformamide (DMF). The UV-VIS spectra showed two main bands – in the UV region and long-wavelength part of the visible spectrum. Structural modifications within the phenyl rings lead to changes in absorption profiles of obtained compounds.

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P032

Fabrication of biobased fibrin-dextran microgels with controlled degradation time via droplet-based microfluidics

Shannon Anna Jung [1,2], Svenja Wein [3,4], Hanna Malyaran [3,5], Caroline Schmidt [1,2], Stephan Rütten [6], Sabine Neuß-Stein [3,4], Andrij Pich [1,2]

[1] *DWI-Leibniz Institute for Interactive Materials, RWTH Aachen, Aachen, Germany*
[2] *Institute for Technical and Macromolecular Chemistry, RWTH Aachen, Aachen*, Germany
[3] *Helmholtz Institute for Biomedical Engineering, BioInterface Group, RWTH Aachen, Aachen, Germany*
[4] *Institute of Pathology, RWTH Aachen, Aachen, Germany*
[5] *Interdisciplinary Centre for Clinical Research, RWTH Aachen, Aachen, Germany,*
[6] *Electron Microscopic Facility University Clinics, RWTH Aachen, Aachen, Germany*

Bio-based materials have gained attention as carriers in biomedical and Tissue-Engineering applications.[1,2] In particular, polysaccharide based microgels are of interest due to their biocompatibility, biodegradability and ability to provide wide variety for functionalization with active groups.[2] However, polysaccharides are not perfectly suited for the encapsulation of growths factors due to the denaturation and suppressed cell proliferation. Contrary, fibrin exhibits high cell affinity, reduced risk of immune response, and can incorporate growth factors.[3] By combining polysaccharides and fibrin as building blocks for design of microgels, it is possible to achieve new properties, e.g. programmed degradation, tuneable mechanical properties and release of growth factors, enabling their application in the Tissue-Engineering.[4]

In this work, bio-based fibrin-dextran-based microgels are synthesized via droplet-based microfluidics with high reproducibility and controlled sizes between 100 – 130 µm. These microgels are produced through two simultaneous processes: a) gelation of fibrinogen with thrombin and b) covalent crosslinking of functionalised dextran. By varying fibrinogen, dextran, and crosslinker amounts and ratios, microgels with different viscoelastic properties and adjustable degradation profiles are obtained. The degradation of microgels is controlled by fibrin-dextran ratio or by the concentration of enzyme dextranase. The loading of the microgels is tested with fluorescein labelled Bovine Serum Albumin protein and the encapsulation and degradation are analyzed with confocal microscopy. The viscoelastic properties of the microgels was determined using nanoindentation. A correlation between the stability, stiffness and degradation time of the microgels could be detected, enabling the prediction of the release of loaded microgels, showing high potential for biomedical applications.

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P033

Nanoscale Surface Photovoltage Spectroscopy (nano-SPV) to study defect densities and the effect of passivation on halide perovskite solar cells

[1,2]Yenal Yalcinkaya, [1]Pascal N. Rohrbeck, [3]Emilia R. Schütz, [3]Azhar Fakharuddin, [3]Lukas Schmidt-Mende, [1,2]Stefan A.L. Weber

[1] Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany
[2] Institute of Physics, Johannes Gutenberg University Mainz, Duesbergweg 10-14, 55128 Mainz, Germany
[3] Department of Physics, University of Konstanz, Universitätsstr. 10, 78464, Germany

Understanding electron and ion dynamics is an important task for improving modern energy materials, such as photovoltaic perovskites. These materials usually have a delicate nano- and micro structure that influences the device parameters. To resolve detailed structure-function relationships on the relevant micro- and nanometer length scales, the current macroscopic and microscopic measurement techniques are often not sufficient.

Here, we introduce nanoscale surface photovoltage spectroscopy (Nano-SPV) and nanoscale ideality factor mapping (Nano-IFM) via time-resolved Kelvin probe force microscopy (tr-KPFM).[1] These methods can map nanoscale variations in charge carrier recombination, ion migration, and defects.[1] To show the potential of Nano-SPV and Nano-IFM, these methods are applied on perovskite samples with different morphologies. A scheme is shown in Fig. 1.[1]

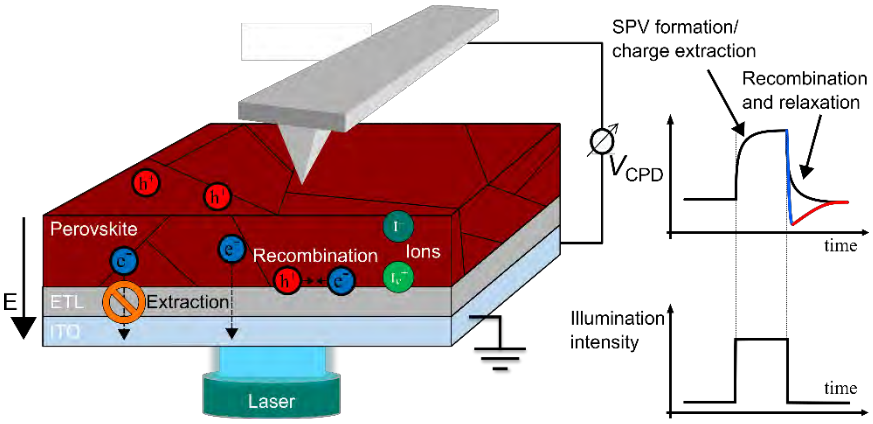

Figure 1: Schematic overview of the tr-KPFM setup. The laser intensity is either modulated in a pulse shape or a slow intensity increase with the tip engaged to the surface while the local CPD signal is recorded. The presence of defect states such as GBs and interfaces hinder the extraction of charges (blocking symbol).

The results clearly show an improved uniformity of the SPV and SPV decay distribution within the perovskite films upon passivation and increasing the grain size. Moreover, Nano-SPV and Nano-IFM could still detect local variations in the defect density, guiding the way for further optimization.

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P034

Synthesis and reactivity of a N-heterocyclic carbene-phosphinidenide manganese carbonyl

Dustin Bockhardt [1], Matthias Tamm [1]

[1] Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Hagenring 30, 38106 Braunschweig, Germany

In the past few years, the chemistry around N-heterocyclic carbene-phosphinidene adducts (‘NHCPA’, NHC=P-R with R = H, Aryl, CN, …) has made significant advances, turning these phosphorus(I) species into an arising class of main group compounds which show numerous reactivities.[1,2] While the transition metal chemistry of NHCPAs as neutral, strongly donating ligands has been explored substantially, NHC-phosphinidenide metal complexes of the type NHC=P-M (M = transition metal) are exceedingly rare.[1] Only a few examples from our group (NHC=P-X with X = (p-Cym)MCl with M = Ru, Os; Cp*MCl with M = Rh, Ir) as well as two complexes of the type $(NHC=P)_2M$ (M = Hg, Mn) are known.[2–6] The former have been successfully used as catalysts for the hydroboration of nitriles, esters and amides.[4]
Herein we present the first diamagnetic 3d-transition metal complex with a terminal NHC-phosphinidenide ligand IDipp=P-$Mn(CO)_4$ (IDipp = N,N’-(diisopropylphenyl)imidazolin-2-ylidene).

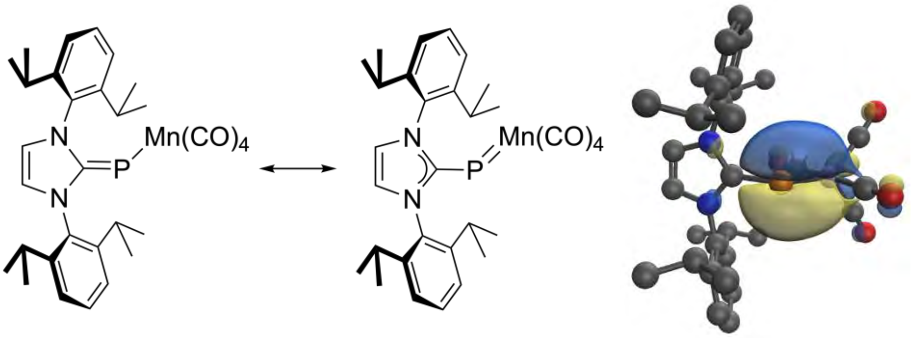

Figure 1: Mesomeric structures (left) of the NHC-phosphinidenide Mn carbonyl and visualization of the Mn=P double bond (right) which corresponds to the HOMO-1 (B3LYP/def2-TZVP).

The P=Mn bond shows substantial double bond character (Figure 1), leaving the metal centre coordinatively unsaturated. Carbonyl ligand exchange as well as the reactivity of the unusual Mn=P bond is studied, envisioning catalytic applications including the splitting of small molecules (e.g., H_2).

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P035

Chemical Upcycling of Polymers into Luminescent Organic Materials

Abdusalom A. Suleymanov[1,2], Kay Severin[1]

[1] *Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, Switzerland*
[2] *Massachusetts Institute of Technology (MIT), Cambridge, USA*

Organic materials with solid state luminescence are useful in chemical sensing, organic light-emitting diodes (OLEDs), bioimaging, and cancer treatment. Tetraarylethenes are popular solid state luminogens. Their preparation usually relies on lengthy multistep synthesis utilizing hazardous conditions and reagents (e.g. *n*BuLi, $TiCl_4$, Pd catalysts).[1]

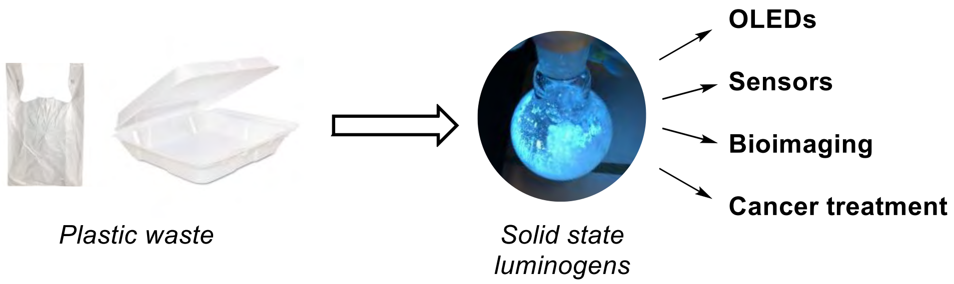

Figure 1: Conversion of plastic waste into valuable solid state luminogens.

We have developed two simple one-step routes to prepare a large variety of tetraarylethenes from commercial starting materials including pharmaceuticals, carbohydrates, peptides, and polymers. Our first method is based on metal-free electrophilic C–H vinylation of aromatic compounds using vinyl triazenes (vinyl cation precursors developed in our laboratory).[2,3] Second method is based on nucleophilic substitution reactions with fluorinated tetraarylethene tags.[1] Importantly, we applied these methodologies for the upcycling of plastics (e.g. polystyrene, polyvinylcarbazole, polyethylene) into valuable solid state luminogens (Figure 1).

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P036

The role of phenylnitrene in the formation of polycyclic aromatic nitrogen containing hydrocarbons

Rahel Arns [1], Rory McClish[2], Patrick Hemberger[3], Andras Bödi[3], Jordy Bouwman[2], Tina Kasper[1], Domenik Schleier[1]

[1] Paderborn University, Chair of Technical Thermodynamics, Paderborn, Germany
[2] University of Colorado Boulder, Institute of Chemistry, Boulder, USA
[3] Paul Scherrer Institut, Laboratory for Synchrotron Radiation and Femtochemistry, Villigen, Switzerland

Chemical energy storage in the form of biofuels is essential for the energy economy of the future. In fields like heavy-duty machines, aviation, or shipping, it is difficult to replace fuels by batteries. Polycyclic aromatic hydrocarbons (PAHs) are a toxic and unwanted side product of combustion processes and understanding their formation is crucial to mitigate their effects. While PAH formation is well studied, potential reactions of nitrogen-rich biofuels[1] leading to polycyclic aromatic nitrogen heterocycles (PANHs) are thus far unknown.

To improve our understanding of the nitrogen chemistry in combustion environments, we investigated the reaction of phenylnitrene with propargyl radicals. Nitrenes are more stable than carbenes, because of their larger singlet-triplet gap[2], and they have been detected in pyrrole and pyridine flames.[3,4] Phenyl azide and 3-iodopropyne were used as precursors to generate the reactive species in a heated tubular microreactor and the products are identified by mass-selected threshold photoelectron spectra (ms-TPES) using double imaging photoelectron photoion coincidence (i2PEPICO) spectroscopy. We performed quantum chemical calculations to gain insights into the chemical pathways leading to reaction products.

We identified the C_9H_7N isomers quinoline, 1H-inden-1-imine and 3-methylene-3H-indole as products in the experiment. The potential energy surface confirms that all of them are formed via addition-elimination reactions that proceed without an entrance barrier. Interestingly, all of the reaction pathways leading to stable products pass through wells that are lower in energy than the final products. While quinoline is the thermodynamically most favourable product, the formation of 3-methylene-3H-indole is kinetically favoured.

Our results show that phenylnitrene is an important precursor for the formation of PANHs. In the comparable reaction of benzyl radicals with propargyl radicals, the only product is naphthalene, the isoelectronic equivalent to quinoline.[5] The presence of the two indene-like products demonstrates the influence of the nitrogen atom.

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P037

Determination of Thermodynamic Properties of Agar with Some Solvents by Inverse Gas Chromatography Method

Sadan Yurtcu Celik[1], Ozlem Yazici[1]

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

Agar is a versatile substance with applications in the food industry, microbiology, pharmaceuticals, cosmetics, and beyond, it is valued for its gelling properties and vegetarian nature.[1] Inverse gas chromatography (IGC) method is easily applicable, low-cost, and provides high-accuracy results. With this method; properties such as surface properties, thermodynamic interaction parameters, glass transition temperature, melting temperature, crystallinity of various materials such as, polymeric materials, clays, liquid crystals cellulosic materials, pharmaceutical materials, dental materials, and composites can be easily determined.[2-4]

In this study, the thermodynamic properties of agar were investigated using the IGC method. The IGC studies were conducted over a temperature range from 373.2 to 398.2 K. In this temperature range, the specific retention volume (V_g^0) values of the solvents were determined by using high boiling point solvents. Then, Flory-Huggins theory polymer-solvent interaction parameters (χ_{12}^{∞}), equation of state theory polymer-solvent interaction parameters (χ_{12}^{*}), weight fraction activity coefficient (Ω_1^{∞}), effective exchange energy parameters (X_{eff}), the partial molar heat of mixing at infinite dilution ($\Delta\overline{\mathrm{H}}_1^{\infty}$), the molar heat of vaporizations of the solvents ($\Delta\overline{\mathrm{H}}_{\mathrm{V}}$), and the partial molar heat of sorption of the solvent ($\Delta\overline{\mathrm{H}}_{\mathrm{S}}$) were calculated.

This research has been supported by Yildiz Technical University Scientific Research Projects Coordination Department. Project Number: FBA-2023-5838

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P038

Responsive block copolymer morphologies through arylazopyrazole photoswitches

Katharina Ziegler [1], Lisa Schlichter [1], Prof. André Gröschel [2], Prof. Bart Jan Ravoo [1]

[1] University of Münster, Organisch-Chemisches Institut, Münster, Germany
[2] University of Bayreuth, Fakultät für Biologie, Chemie und Geowissenschaften, Bayreuth, Germany

Supramolecular structures that can reversibly change their shape are of great interest for the development of intelligent materials [1] In this project, light-responsive polymers capable of forming different aggregates in aqueous solution were prepared. Amphiphilic block copolymers with varying block lengths were synthesized via reversible-addition-fragmentation-chain-transfer (RAFT) polymerization. Our polymers can self-assemble in water and form different supramolecular morphologies as micellar or wormlike structures. The hydrophilic block consists of water-soluble poly(oligo(ethylene glycol)) methacrylate (POEGMA), while the hydrophobic part contains an arylazopyrazole (AAP) derivative as a photoswitch.[2] By incorporating the light-responsive AAP into the block copolymer, the hydrophobicity of the block chain can be changed by irradiation with green light (520 nm, E-isomer) and UV light (365 nm, Z-isomer). The AAP in the polymer could be reversibly switched from E- to Z-state over various cycles. The configuration of the AAP also influences the aggregation behaviour of the polymers. Using different self-assembly methods different morphologies could be achieved depending on the isomerization state of the AAP in the block copolymer. So, the polymer containing the E-isomer can form micelles, while the one containing the Z-isomer wormlike structures could be obtained. In addition, the morphology of the polymer can be changed even after assembly from micellar to wormlike structure while irradiating with UV-light and vice versa by irradiation with green light.

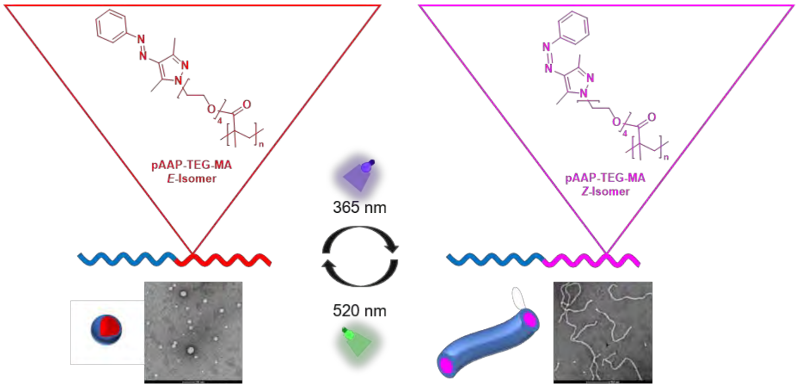

Figure 1: Light-responsive polymer system, assembling to different supramolecular structures dependent on configuration of the AAP in the hydrophilic block of the amphiphilic block copolymer.

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P039

New aza-BODIPY derivative chelating boron – Synthesis and spectral properties

Aleksandra Pawska [1], Michal Kryjewski [1], Barbara Wicher [2]

[1] Chair and Department of Inorganic and Analytical Chemistry, Rokietnicka 3, 60-806 Poznan, Poznan University of Medical Sciences, Poland.
[2] Department of Chemical Technology of Drugs Grunwaldzka 6, 60-780 Poznan, Poznan University of Medical Sciences, Poland

BODIPY (***bo**ron **dipy**rromethene)* and their analogues – aza-BODIPY are compounds that are under intense investigation for their fluorescent properties. Moreover, they represent a new class of photosensitizers used in photodynamic therapy (PDT). PDT is an effective treatment for many diseases, including cancer. In this method, a photosensitizer (PS) generates reactive oxygen species when exposed to the appropriate wavelength.[1,2]

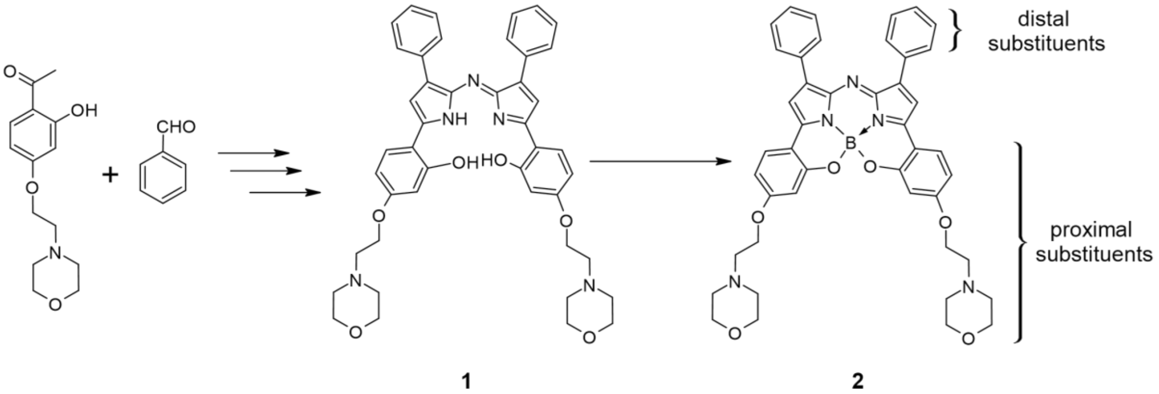

Figure 1: Synthesis of aza-BODIPY with bulky proximal substituents

Several steps in the synthesis yielded azadipyrromethene (1, Fig. 1), which contains hydroxyl groups at the ortho positions of the proximal substituents. Subsequent complexation reaction using boron trifluoride gave compound 2, which belongs to the aza-BODIPY group. Compound 2 is characterized by absorption of light in the near-infrared range (λ_{max} > 750 nm), which is desirable for PDT.

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P040

Glycosylated Carbazole-BODIPY-GO Nanocomposites for Targeted Photodynamic Therapy

Ümm g kpolat[1], Ezel Özt nd z[1], Elif Okutan[1]

[1] *Gebze Technical University, Department of Chemistry, Gebze, Kocaeli,41400, rkiye*

According to WHO cancer related death is one of the leading causes of death with increasing economic and social burden in all over the world. Chemotherapy is still holding the leading position in cancer therapies which comes with the strong cytotoxic and side effects. Lately therapy strategies based on combination of two or more methods has been reputed to reduce the side effects with better efficiency. Combination of chemotherapy with photo dynamic therapy (PDT) is one of the preferred strategies where the PDT is a non-invasive therapeutic modality works with light, molecular oxygen, and photosensitizer (PS). BODIPY chromophores are widely employed as ideal whereas integration of BODIPYs with pharmacologically active molecules like carbazole and nanosized vehicles such as graphene oxide may overcome the limiting efficacy of PDT[1,2].

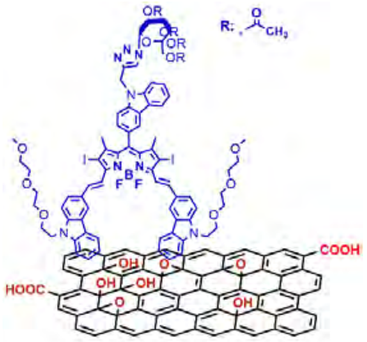

Figure 1: Carbazole-BODIPY-GO based nanocarriers.

Herein, tumour targeted carbazole-BODIPY-GO nanocarier as triplet photosensitizer was prepared, and characterized via mass spectrometry, ^{1}H ^{13}C NMR, Raman and FT-IR analysis. Morphological features of the molecules were investigated via TEM analysis. The photophysical properties and the ability to produce singlet oxygen via indirect method under light were investigated.

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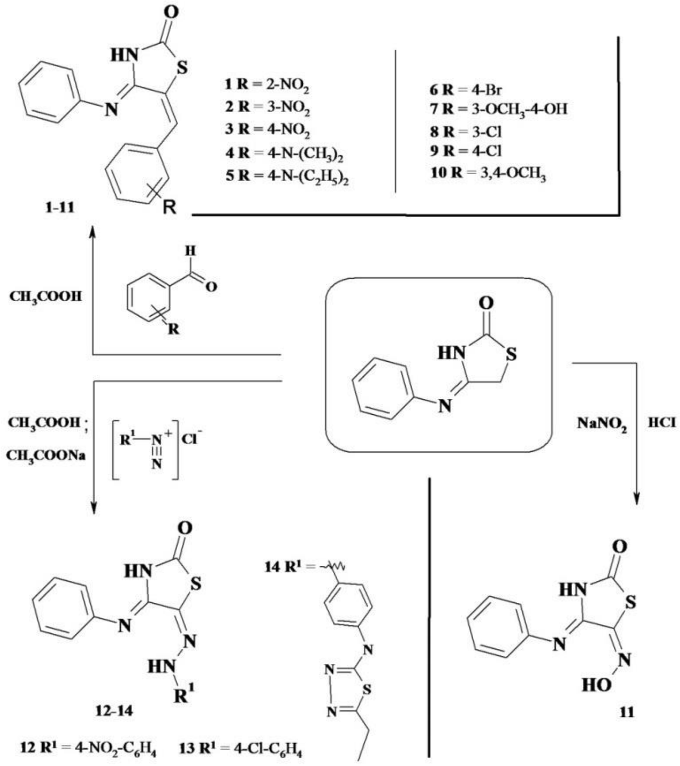
P041

Anti-inflammatory activity of some 4-phenylimino-thiazolidin-2-ones

Maxym T. Khanas[1], Zoriana I. Chulovska [1], Taras I. Chaban [1], Iryna V. Drapak [1], Ihor G. Chaban[1], Olena. V. Klenina [1], Volodymyr V. Ogurtsov [1]

[1] *Danylo Halytsky Lviv National Medical University, Lviv, Ukraine*

Organic heterocyclic compounds currently account for about 70 % of all clinically used drugs. Thiazolidinones are one of the most intensively investigated classes non-condensed heterocyclic systems. They are a biologically important five-membered compounds possessing practically all types of pharmacological activities. 4-Iminothiazolidones, in simile with isomeric 2-imino derivatives, are have been deficiency studied. In this work, which is the portion of our exploring biologically active heterocycles we synthesized a series of C^5 substituted 4-phenylimino-thiazolidin-2-ones for pharmacological screening of anti-inflammatory activity. Literature survey data showed that the interaction of 4-iminothiazolidin-2-one with aniline allows to obtained 4-phenylimino-thiazolidin-2-one. The specified scaffold represents a convenient intermediate in order to afford C^5 substituteds 4-phenylimino-thiazolidin-2-ones. The active methylene group presence in C^5 position of the basic scaffold provides an entry for its utilization in Knoevenagel condensation, nitrosation and azo coupling reactions leading to appropriate 5-arylidene, 5-oxime and 5-aryl-hydrazono derivatives of 4-phenylimino-thiazolidin-2-one generation (**1-13**).



In vivo studies of the exudative phase inflammation was executed based on the functional model of carrageenan-induced rat paw edema . For comparison, the anti-inflammatory activity of a famous anti-inflammatory drug – Ibuprofen in average therapeutic doses was studied in similar conditions. The obtained results of the performed anti-inflammatory activity evaluation have shown that synthesized compounds have expressive anti-inflammatory properties and some of them approach or prevail the Ibuprofen in terms of activity. [1]

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P042

Investigation of Multicomponent Equimolar Rare Earth Zirconates as Thermal Barrier Coatings

Manuel Schenker [1], Maren Lepple [1]

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

Thermal Barrier Coatings (TBCs) are used in turbines as insulator to overcome the temperature limitations of the metallic engine components. The efficiency of a turbine depends proportional on the combustion temperature of the fuel. Higher working temperatures can therefore minimise the fossil fuel consumption. The development of the working temperature in airplane turbines over the last decades is shown in Figure 1.

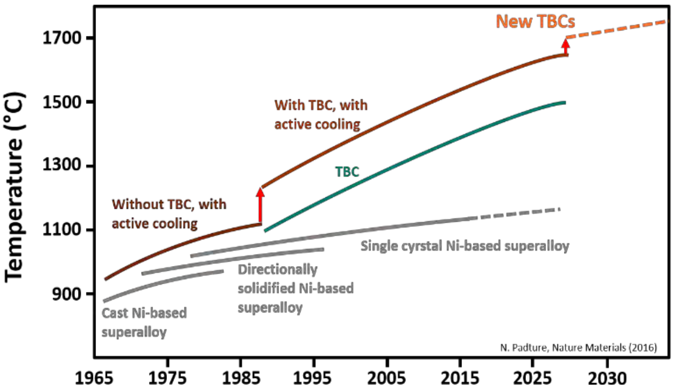

Figure 1: Development of temperature capabilities in turbines in the past decades adapted from *Padture*.[1]

High entropy oxides (HEOs) are investigated as promising material for TBC application. *Rost et al.* synthesised $(Mg_{0.2}Ni_{0.2}Co_{0.2}Cu_{0.2}Zn_{0.2})O$ as the first HEO in 2015.[2] The high configurational entropy results in a high temperature stability due to the entropy term in Gibbs-equation. Furthermore, the high disorder leads to a increased phonon scattering resulting in a low thermal conductivity.[3] Besides that, a TBC needs to have a coefficient of thermal expansion that is close to that of the metallic substrate. Phase stability in a large temperature range is required due to the cyclic thermal conditions in an aircraft turbine.

The focus of the project is to investigate the thermocyclic behaviour of high entropy TBCs (based on rare earth zirconates) with a laser-rig to determine the lifetime of the coatings. A laser-rig is used instead of an oven due to a settable temperature gradient which can be obtained with such setup, and which is closer to the conditions inside a turbine. Additionally, a laser enables a wider temperature range that can be investigated compared to a burner-rig.

Acknowledgements:

The work is funded by German Federal Ministry of Education and Research (03XP00301).

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P043

In situ monitoring of electroactive biofilms with low frequency torsional QCM-D devices

Carl Schneider[1], Diethelm Johannsmann[2], Uwe Schröder[1]

[1] *University of Greifswald, Institute of Biochemistry, Greifswald, Germany*
[2] *Clausthal University of Technology, Institute of Physical Chemistry, Clausthal-Zellerfeld, Germany*

Using electroactive biofilms in microbial fuel cells (MFCs) shows great promise for turning wastewater management from an electricity intensive industry into a renewable power source.[1] Monitoring the growth of these biofilms *in situ* proved challenging in the past and still does so today. Gaining information about the dependence of their electrical performance on biomass as well as stress responses has been an ongoing topic of research and discussion. Continuing the work of Sievers et al.[2,3] the effectiveness of a novel method for *in situ* characterizations using low-frequency torsional quartz crystal microbalances with dissipation monitoring (QCM-D) was shown. This promises deeper views into internal processes of these biofilms than regular QCM-D devices.

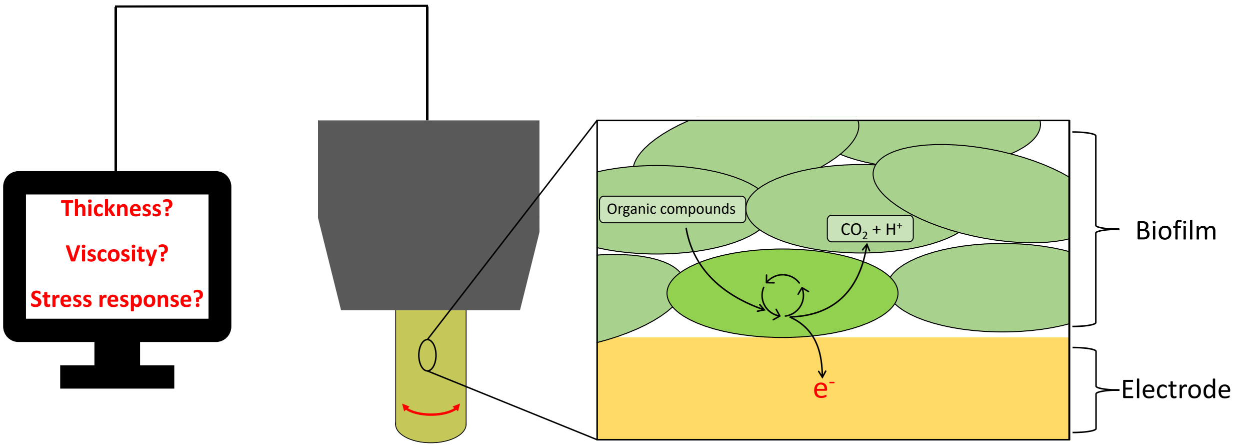

Figure 1: Schematic depiction of torsional resonators and cultivated electroactive Geobacter spp. biofilm.

The study presented here supported previous findings that torsional QCM-D devices are suitable for monitoring growth and stress responses of electroactive *Geobacter spp.* biofilms. Biofilms up to thicknesses of ≈ 40 µm could reliably be monitored. During initial development, investigations showed a linear correlation of current densities produced and biofilm thickness, i.e., biomass. Viscoelastic parameters, in case of this study viscosity, were also found to have strong linear correlations with measured current densities. This suggests these parameters to be affecting the performance of MFC devices, and their consideration being crucial when working towards wide-scale implementation.

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P044

Engineering bacterial interactions with photoactive electrospun materials: role of photosensitizer charge and fiber diameter on activity

Fabian Terlau [1], Anzhela Galstyan [1,2]

[1] University Duisburg-Essen, Institute of Chemistry, 45141 Essen, Germany
[2] Center for Nanointegration Duisburg-Essen, Centre for Water and Environmental Research and Center for Medicinal Biotechnology (ZMB), 45141 Essen, Germany

Antimicrobial photodynamic therapy (aPDT) has emerged as one of the attractive alternatives to antibiotics for treatment of bacterial infections.[1] Reactive oxygen species (ROS) formed through energy or electron transfer from the triplet state of excited photosensitizers (PS) are able to inactivate microbes very efficiently.[2] There are numerous studies on application of PS solution at the infected area.[3] However, when the PS is embedded in solid support (e.g. water filters) durability and consequently the antimicrobial effect are enhanced.[4] Fibrous membranes for PS immobilization can be easily created through the electrospinning process, a reliable method to create a vast variety of membranes since a wide selection of different polymers can be used, enabling control of different characteristics of the final product (e.g. fiber diameter, hydrophilicity).[5]

The overall antimicrobial effectiveness of such materials is influenced by many parameters such as PS properties (e.g. fluorescence lifetime, polarity) or surface characteristics (e.g. antifouling properties).[4] A wide variety of different PS and polymer membrane combinations were investigated in literature.[4] Nonetheless, parameter optimization for the membranes themselves was rarely conducted. In this study we used the class of phthalocyanines as PS to investigate the influence of fiber diameters and PS polarity on antimicrobial activity. Further, the difference between covalently bound and lose PS will be investigated.

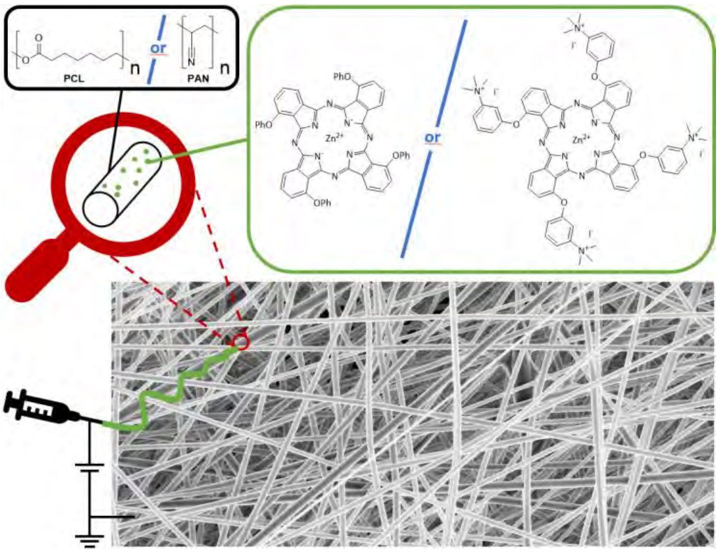

Figure 1. Design of photodynamically active elcectrospun materials and chemical structures of selected PS and polymers used in this study.

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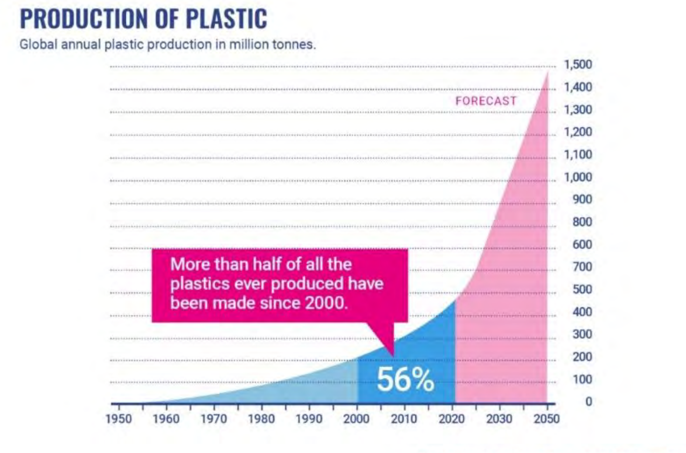
P045

Depolymerisation of Poly(propylene carbonate)

Nicole Dickmann [1], Prof. Dr. Thomas Werner [1], Prof. Dr. Matthias Bauer [1]

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

The increasing population becomes a growing problem for our environment. The high demand for resources is accompanied by an ever-growing amount of waste products. One of the biggest pollutants in our environment is post-consumer plastic waste. Due to incorrect disposal of waste up to 12.7 million tons of plastic end up in our oceans each year, killing thousands of animals and destroying maritime habitats.[1] For these reasons it is an important task to remove those waste materials and dispose them in an environmentally friendly way.



SOURCE: PLASTIC ATLAS, ASIA EDITION, 2021 | © PLASTIC SOUP FOUNDATION

Figure 1: Global Production of plastic.[2]

The optimal disposal of post-consumer plastic would be its depolymerisation to obtain valuable chemicals and achieve a circular economy. In this work the depolymerisation of poly(propylene carbonate) is investigated. To obtain a high yield of valuable chemicals transition metal catalysts are often used, such as Cr[3] catalysts. Due to the toxicity and non-environmentally friendly properties, it is worthwhile to find suitable alternatives, such as base initiated depolymerisation. The optimisation of this reaction could lead to the production of at least three different valuable products in different ratios. With this method the formation of each product could be controlled by changing the reaction conditions leading to a circular economy, which can easily be modified to meet changing demands.

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P046

Antibacterial Textile Coating

Şevval Akın [1], MSc.Emine Yıldırım [2], Prof.Dr. Melda Altıkatoğlu Yapaöz[1], Prof. Dr. Tarık Eren [1]

[1] Yıldız Technical University, Faculty of Art and Science, Chemistry Department
Istanbul,Turkiye
[2] Organic Chemistry Industry and Trade Joint Stock Company
Istanbul,Turkiye

Bacterial infections is growing problem and lead to the spread of infectious diseases and an increase in mortality rates. [1] The development of antibacterial materials is one of the key strategy against to combat bacteria infection. The textile materials we use in our daily lives are not antibacterial.[2] Silver-based compounds are generally used to obtain antibacterial properties. However, silver is leached out from the surface over time and with washing cycle, causing the surface to lose its antibacterial properties.

Here, a quaternary ammonium salt bearing polyvinyl pyridine and chitosan were synthesizedand the used to coat the textile surface. [3-4] To enhance the antibacterial efficacy, different hydrophobic tail groups and silver salts were used in the formulation to obtain a polymer-nanoparticle-based biocidal coating showing dual action against bacteria. The surface biocidal efficacy of the material was tested against E. coli and S. aureus bacteria.

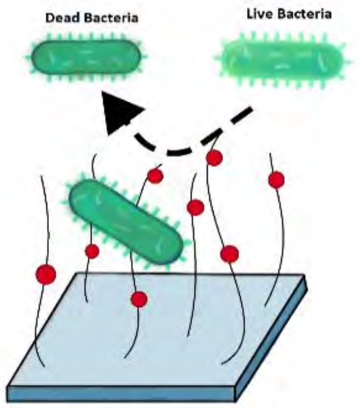

Figure 1: Textile-bonded contact killer coating

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P047

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

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

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

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

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

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

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

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P048

Triphenylamine Substituted Asymmetric Zinc Phthalocyanines as Alternative HTL for Perovskite Solar Cells

Gizem GÜMÜŞGÖZ ÇELİK[1], Muhittin ÜNAL[2], Seçkin AKIN[2], Ayşe G I GÜREK[1]

[1]Gebze Technical University, Department of Chemistry, Kocaeli, Turkey
[2]Necmettin Erbakan University, Department of Metallurgical and Materials Engineering, Konya, Turkey

Perovskite solar cells (PSCs) have emerged as a promising renewable energy source due to their high efficiency, low costs and simple fabrication by solution-processing methods. However, the stability of PSCs is one of the major obstacles to their commercialization [1]. The hole transport layer (HTL) plays a critical role in stability. The HTL must support the adequate movement of charges and protect the perovskite layer from environmental conditions. The commonly used HTL material is spiro-OMeTAD, which has high electrical conductivity, but it does not provide adequate stability to PSCs and is quite expensive. Less expensive molecular materials, such as metal phthalocyanines, are a good alternative for PSCs because they provide more stability than spiro-OMeTAD[2] .

In this study, two different asymmetric phthalocyanine compounds containing tert-butyl groups and a triphenylamine group, were synthesized, characterized, and their optical and electrochemical properties were investigated. To investigate their behaviour as hole transport material (HTM), ***asym-ZnPc*** and ***asym-O-ZnPc*** were produced in the cell architecture given in Figure 1 and compared with spiro-OMETAD.

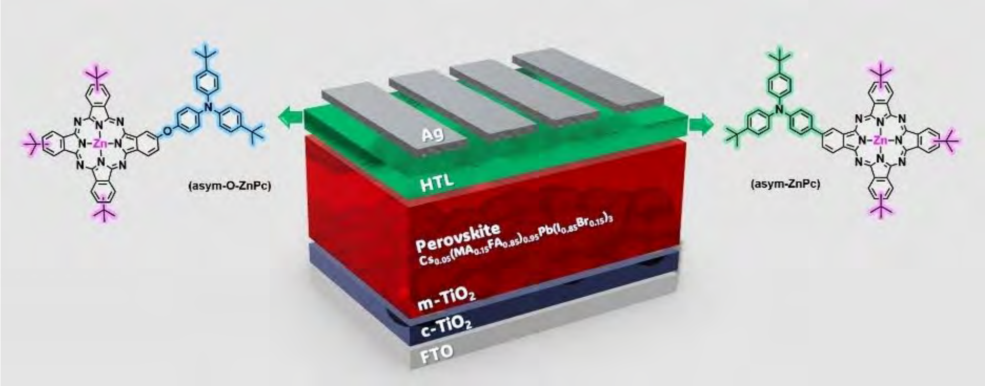

Figure 1: Device architecture of PSCs.

To determine the performance of cells, I-V characteristics, TRPL measurements and stability profile determination studies were carried out in a 40-45% relative humidity environment. The results showed that asym-ZnPc and asym-O-ZnPc exhibited better stability than spiro-OMETAD.

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P049

CeO_2 NR cocatalized Ni and NiCu anode electrocatalysts for EOR

Emine Sena Kazan-Kaya[1], Mahmut Bayramoğlu [1]

[1] *Gebze Technical University, Chemical Engineering Department, Kocaeli, Türkiye*

Ethanol is one of the most promising, non-hazardous, and affordable alternative fuels; however, in order to convert ethanol into energy, the ethanol electrooxidation reaction (EOR) must be carried out effectively. Unfortunately, due to the slow kinetics of EOR, this clean alternative fuel cannot be used on a commercial scale.[1] To increase EOR kinetics, an effective and stable anode electrocatalyst needs to be synthesized.In this study, effective anode electrocatalysts for EOR were synthesized using Ni and NiCu nanoparticles co-catalyzed with CeO2 nanorods (NRs). Morphological characterizations of the synthesized electrocatalysts were performed by XRD, SEM, TEM and XPS analyses, and the results showed that the electrocatalysts were successfully synthesized. The catalysts were subjected to electrochemical characterizations using Chronoamperometry (CA), Linear Scan Voltammetry (LSV) and Cyclic Voltammetry (CV) methods. Figure 1 shows the CV results of the electrocatalysts synthesized in 1M Ethanol + 0.05M KOH solution.

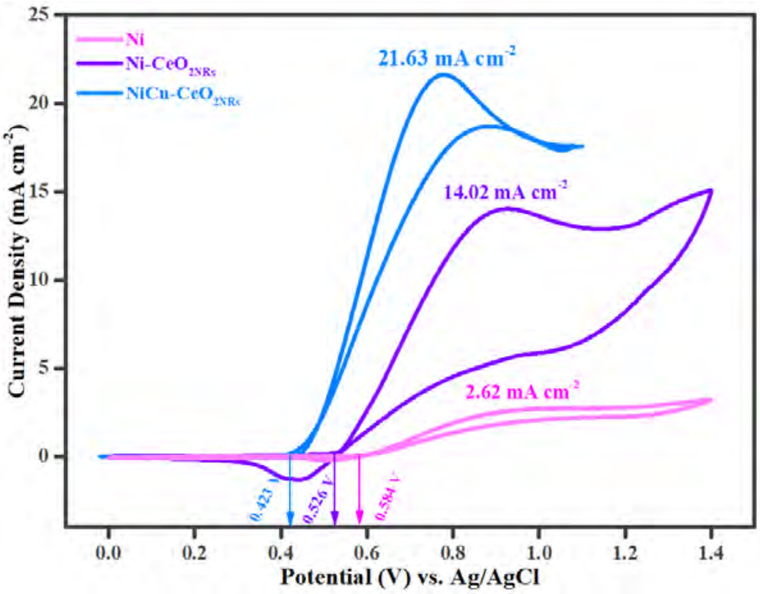

Figure 1: The CV voltammograms of Ni, $\text{Ni-CeO}_{2\text{-NRs}}$, and $\text{Ni-CeO}_{2\text{-NRs}}$ electrocatalysts in 0.05M KOH + 1M Ethanol; 0.01 V s^{-1} scan rate.

Accordingly, adding CeO_2 NRs to pristine Ni resulted in a negative shift in onset potentials and higher current density, indicating better catalytic activity.[2] Also, the addition of copper to nickel enhances the synergistic effect, resulting in broader oxidation peaks. This increase in current density further supports the presence of a synergistic effect between Cu and Ni, promoting EOR, the CeO_2 NRs in the catalyst plays a crucial role in enhancing the synergistic effect.

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P050

Synthesis of multivalent oligomannosyl glycopeptide conjugates as potential HIV vaccine candidates

Anurag Roy [1], Mahesh Neralkar [1], Isaac J. Krauss [1]

[1] *Brandeis University, Waltham, USA*

Carbohydrate based vaccines have prominent pharmaceutical importance against a diverse array of bacterial and viral infections, as well as HIV. Broadly neutralizing antibodies (bnAb) such as 2G12, PGT128 and PGT122 bind tightly to the heavily glycosylated “high-mannose patch” on gp120 protein of the HIV virion and neutralize a broad range of HIV strains which plays a significant importance in the development of vaccines for HIV. The Krauss lab employs a novel directed evolution method to discover glycopeptide sequences that mimic the epitopes of these antibodies.[1] A major barrier in carbohydrate-based HIV vaccine development is the serum mannosidase trimming of terminal mannose “tips” from the $Man_9GlcNAc_2$ glycan, which directs the antibody response towards the undesired glycan core instead of the tips.[2]

A possible solution to this problem is chemical stabilization of the Manα1->2Man linkage against this enzymatic hydrolysis by using sulfur in the glycosidic linkage for the Manα1->2Man termini in the Man_9-glycans.[3] This work reports a plausible pathway to chemically synthesize serum stable $Man_9GlcNAc_2$-glycopeptide conjugates bearing the S-linked Manα1->2Man linkage, and their binding affinity studies with different HIV bnAbs. Another aspect of this research is the chemical synthesis of the different peptide sequences which are selected via the directed evolution method against a particular HIV bnAb and determining their binding affinity as well as in-vivo immunization stability. The “hits” arising from this research can direct us to suitable lead vaccine candidates, to be tested for antibody generation in vivo.

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P051

Supramolecular Polymer Coatings based on Peptide Self-Assembly

Mahdi Samapour [1], Sebastian B. Beil [1]

[1] *University of Groningen, Stratingh Institute for Chemistry, Groningen, Netherlands*

Climate change is one of the main issues of today's world; to deal with this issue, governments set up the Paris Agreement to control it with various solutions like the circular economy; one of the key parameters for achieving the circular economy is recycling of existing materials [1], and coating is among of them but according to the American Coating Association many industrials coatings lack recyclability, and also most of these traditional coatings lack of responsiveness. So, we aim to develop responsive bio-based coatings to be “smart” and “recyclable” alternatives. External stimuli (pH, ions, or mechanical stress) can cause structural changes to the coatings and thus induce a visible color change. Moreover, these coatings can act as a selective permeable membrane for chemicals or gases like H2O, O2, etc. [2]

The responsiveness of the polymer coatings can be tailored by modifying the assembly protocol and finetuning of the building block structures. [3]

Taking advantage of the modularity of our coatings that contain a hydrophobic polymer (yellow), a crystalline motif (green), and a sensitizing unit (purple), we can easily design various types of novel responsive coatings. The supramolecular nature of the assembled coating enables a higher degree of recyclability already in the initial design.

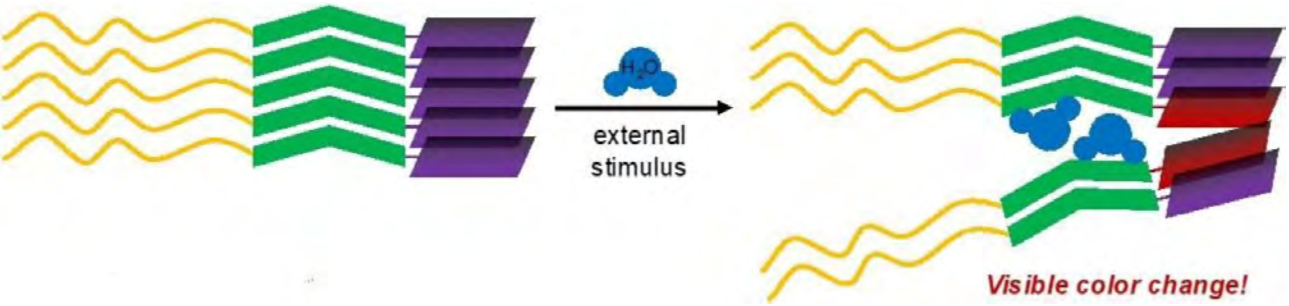

Figure 1: Smart coating design

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Evaluation of the Integration of a New Trend Energy Generation System into Wastewater Treatment Plants Using Energy and Exergy Analysis

Hatice Kubra Erdogan [1], Bestami Ozkaya [1]

[1] Yildiz Technical University, Faculty of Civil Engineering, Department of Environmental Engineering, Istanbul, Turkey

Wastewater production is increasing rapidly with urbanization and population growth, especially in developing countries. A significant portion of the energy consumption at the global level is due to the energy need for wastewater treatment processes [1-2]. With increasing global climate concerns, energy conservation, energy efficiency and energy substitution have become a common development principle adopted worldwide [3]. Given the abundance and ease of access, together with the characteristics of wastewater content, it can be considered as a promising source of hydrogen [1]. The integration of systems capable of producing hydrogen in the wastewater treatment process not only reduces greenhouse gas emissions, but also plays a critical role in terms of recovering the energy spent for treatment [4]. Improvement of existing systems and energy saving measures in wastewater treatment plants can significantly reduce energy requirements. In this context, energy and exergy analysis stands out as a critical tool to ensure the sustainability of wastewater treatment systems and to increase energy efficiency. [5-6].

In this study, a thermodynamic analysis was performed based on the information obtained from a wastewater treatment plant. In order to analyze the efficiency of the wastewater treatment plant system, the plant processes are modeled based on energy and exergy parameters. The data of the system were analyzed with the EES (Engineering Equation Solver) program. Finally, the potential of meeting the electricity demand of the plant by integrating the biological hydrogen production method taken as a reference into the advanced biological wastewater treatment plant is examined.

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P053

The Thermal Behaviour of Double-Walled Phase-Change Microcapsules (PCMs)

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

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

Energy storage has a remarkable effect on achieving supply and demand balance for energy.[1] Phase change materials (PCMs) could absorb or release large amounts of heat during the phase change process, they have attracted a lot of attention in the energy sector.[2] PCMs are used extensively in thermal management systems, such as solar heat storage, heat exchangers, building insulation materials.[3] However, optimization a stable environment in which the PCM can undergo its phase change without leakage and high thermal conductivity for a long time is one of the requirements for the end product usage.

Here, commercially available PCM PX-25 (RUBITHERM®) was further coated with silica or carboxymethyl cellulose to enhance the mechanical stiffness of the capsule layer and increasing long term usage in the application process. (Figure 1) Microcapsules was developed through a dip coating and spray coating techniques. The heat storage efficiency of the double layer PCM was then investigated using heat storage tests.

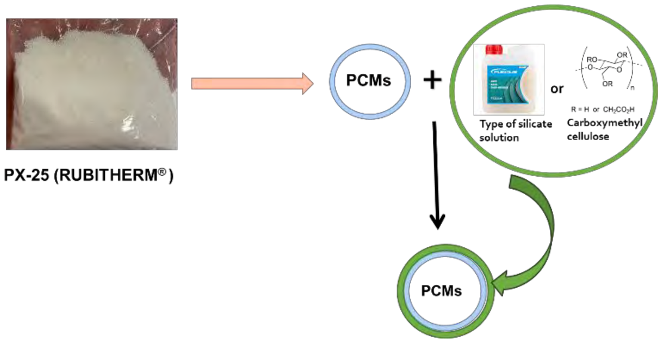

Figure 1: Coating of commercial encapsulated silica core PCMs (PX-25 RUBITHERM®) with silica or carboxymethyl cellulose

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P054a

Events of the JCF Münster - What we do

Luca Peters [1]

[1] *University of Münster, Department of Chemistry, 48149 Münster, Germany*

The JCF Münster offers students at the University of Münster numerous opportunities to take a look at academic and industrial life. Every year we offer the "Chemistry-industry-forum" (ChInFEo), which is aimed at students and PhD students. With companies from different areas of industry, we welcome all interested parties. With short presentations, the companies can introduce themselves and give students and PhD students a first impression.

Every year, in cooperation with Evonik Industries AG, we award the Evonik Prize for outstanding achievements in master's and doctoral theses. The prizes are endowed with 500 and 750 euros. Proposals are submitted by the professors but can also be submitted by students. At the award ceremony, Evonik will give a short presentation, followed by the laudatory speeches and award presentations. This will be followed by a lecture and a get-together.

In addition, we organize the "Career paths of Münster chemists" where 3-4 alumni of the University of Münster report on their career entry. After short presentations, the alumni will be available to answer questions about the application process, their companies, etc.

Q.Uni is aimed at the University of Münster's children's and youth university. With an exciting show to marvel at and take part in, we give children and young people a first insight into the world of chemistry.

The "Industrial internship in chemistry studies!?" students report to students about their industrial internships. After a round of introductions and short presentations, the stage is open for questions.

The JCF Münster also takes part in the department's summer party, which is organized together with the student council, the young food chemistry and young biochemistry students. The JCF is organizing an interesting lecture. Afterwards, there will be a barbecue with cool drinks on the university grounds.

P054b

Events on careers & Internships

Jan C. Spies [1]

[1] *Universität Münster, Institute of Organic Chemistry, Münster, Germany*

One of the goals of the JCF Münster is to provide chemistry students with I insight that goes beyond academic life. For this reason, we hold two events annually, one being the “Career paths of chemists from Münster” and the other being “Industry Internship?!”.

The first event, “Career paths of chemists from Münster”, is targeted at all students and aims at giving them a better understanding of how their own career might look like after finishing their studies in Münster. To do this, we invite alumni that have recently started their professional careers. We put special focus on inviting alumni with different careers, ranging from lab management in the chemical industry to consulting and even less common jobs. Aside from giving an overview over their career path, each speaker will also talk about their application process, especially for their first job. We also try to include alumni that started their professional careers directly after their master thesis. In general, our goal is to give broad perspective on the various career options that one has after studying chemistry.

The second event, “Industry Internship?!”, is especially targeted at Bachelor and Master students, who consider conducting an internship in industry. As an internship in a research institute abroad is the norm for chemistry students in Münster, conducting an (additional) internship in industry is a decision many students struggle with. Our event is supposed to help those students with exactly that by letting older students, who did do exactly such an internship, talk about their experiences.

Both events have one big advantage that other sources of information like job fairs do not possess. In both (former) students are the presenters which removes a big barrier to ask even personal questions about each unique experience that would otherwise not be asked. These events are therefore very popular and help to connect younger students with older students and alumni so they can gain from their experience.

P054c

The Evonik Prize of the JCF Münster

Caroline Witter [1]

[1] *University of Münster, Department of Inorganic Chemistry, 48149 Münster, Germany*

The Evonik Prize is an annual event organized by the JCF Münster in cooperation with Evonik and the professors of the Department of Chemistry. The prize is awarded to outstanding master's or doctoral theses and is also endowed with prize money. Professors and students can propose candidates and a jury, consisting of professors from the respective institutes, evaluates the applicants based on various criteria.

The award ceremony with laudatory speech will be rounded off by a presentation by Evonik and a guest lecture. Afterwards, there will be a get-together with drinks and pretzels to encourage an exchange between award winners, professors, guest speakers and Evonik.

This well-established event is always an opportunity to promote our regional group. We are grateful to have Evonik, a long-standing cooperation partner and sponsor, at our side. We hope that this will inspire other JCFs to initiate similar projects.

P055

Studies towards the 12-membered ring system of the calyculones from the octocoral *Eunicea calyculata*

Vincent Malecha, Thomas Lindel

TU Braunschweig, Institute of Organic Chemistry, Braunschweig, Germany

The cubitanoids calyculone A (**1**), B and C where first isolated from the Caribbean octocoral *Eunicea calyculata* in 1984 and later expanded by calyculones D-G (1991) and H-I (2012).[1-3] They belong to a small group of 12-membered monocyclic diterpenes sharing the cubitane framework **2** of (+)-cubitene (**3**). While most of the calyculones are marginally active against tuberculosis and malaria, calyculone A (**1**) also showed cytotoxicity (GI_{50} = 194 nM, 18.8 nM and 284 nM, NCI USA) against SR leukemia, RFX 393 renal cancer, and UACC-62 melanoma, potentially qualifying calyculone A (**1**) for a therapeutic application.[3]

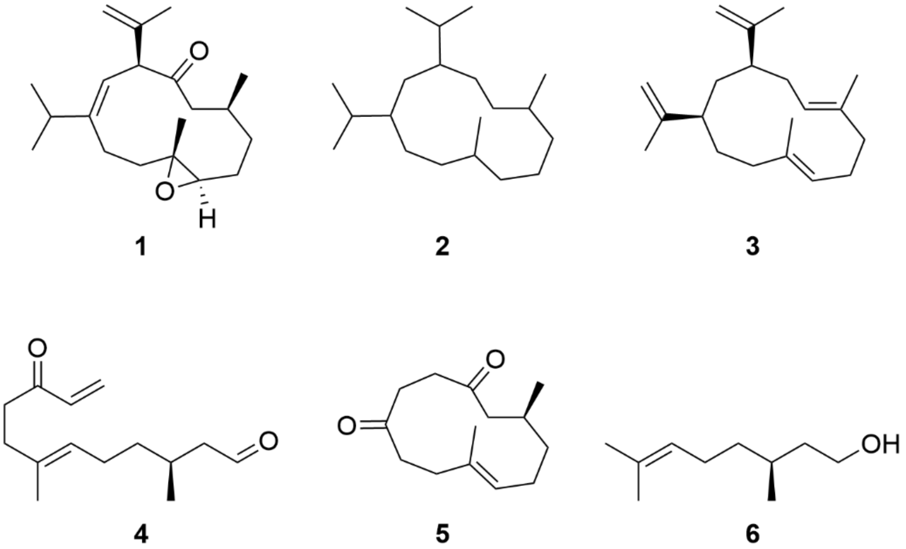

Figure 1: Structures of calyculone A (**1**), the cubitane framework **2**, (+)-cubitene (**3**), dienal **4**, 1,4-diketone **5** and (*S*)-citronellol (**6**).

To date, no total synthesis of any of the calyculones has been achieved. Previous studies concluded that the formation of the 12-membered ring is the most challenging task.[4] In a model study, we address the synthesis and ring closure of dienal **4**, ideally affording 1,4-diketone **5**. In particular, carbene catalysts that form Breslow-type intermediates are under investigation. The use of samarium diiodide is another option that may open up a reductive radical addition pathway. (*S*)-citronellol (**6**) is employed as a starting material in a chiral pool approach.

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P056

Shape-anisotropic palladium nanoparticles synthesized hydrothermally on polyurethane sponges for heterogeneous catalysis

Lisa C. Bernhard [1], Olivier Gazil [1,2], Miriam M. Unterlass [1,3]

[1] University of Konstanz, Department of Chemistry, Konstanz, Germany
[2] Polytechnique Montreal, CREPEC, Montreal, Canada
[3] CeMM Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria

Elemental Palladium (Pd) is an extremely useful hydrogenation catalyst.[1][2] Of particular relevance for catalysis are Pd nanoparticles (NPs), as they provide a higher portion of surface atoms, which enable said activity in hydrogenation, than bulk Pd. Synthetically one typically reduces Pd salts, commonly Na_2PdCl_4, in solution in the presence of ligands or surfactants, which stabilize the formed NPs through coordinating to their surface. As for any metal NPs used for catalysis, catalytic selectivities of Pd NPs can be tuned through the particle morphology, i.e., through growing particles that feature a higher proportion of the catalytically highly active nanocrystal loci vs. the less active facets, in other words: by generating shape-anisotropic Pd NPs. For synthesizing shape-anisotropic Pd NPs, one typically employs seed particles in the presence of surfactants and capping agents, which block crystal growth on specific facets.[1] Furthermore, for technical application, the Pd NPs have to be anchored on a support (e.g., metal oxides)[2] in order to (i) enable reusability (especially compared to the difficult recovery of NPs dispersed in solution), and (ii) enable operation in flow (by loading into a reactor). We have recently developed a hydrothermal synthesis of near-spherical noble metal NPs anchored on a polyurethane foam (PUF).[3]

Here, we expand on the reported Pd NP@PUF systems, specifically with respect to accessing shape-anisotropic Pd NPs. We show that under hydrothermal conditions anchored anisotropic Pd NPs can be generated using different surfactants in the presence of the PUF. Inductive coupled plasma - optical emission spectroscopy (ICP-OES) were employed to characterize the amount of Pd on the PUF support, while transmission electron microscopy (TEM) was used to determine size and shape of the NPs. Furthermore, for assessing the catalytic properties of the Pd NP@PUF materials, we determined the turnover number (TON) and frequency (TOF) for a model hydrogenation, which was performed in a fully automated setup and its progress was monitored by UV-Vis spectroscopy. Particular attention has been placed on evaluating the effect of Pd NPs' size and morphology on the reaction kinetics. Furthermore, we tested the Pd NP@PUF materials as cross-coupling catalysts and monitored their functioning via nuclear magnetic resonance (NMR) spectroscopy. We here provide an environmentally friendly alternative for generating anisometric Pd NPs on porous supports and evaluate their use as recyclable catalyst.

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P057

In-depth chemical analysis and exposure assessment of crumb rubbers in artificial turf

Madison H. McMinn [1], Katherine Poisson [1], Paola Pimentel [1], Pranali Ashara [1], Xinwen Zhang [1], Jessica Eig [1], Loretta Fernandez [2,3], Zhenyu Tian [1,3,4]

[1] Northeastern University, Department of Chemistry and Chemical Biology, Boston, USA
[2] Northeastern University, Department of Civil and Environmental Engineering, Boston, USA
[3] Northeastern University, Department of Marine and Environmental Science, Boston, USA
[4] Northeastern University, Barnett Institute for Chemical and Biological Analysis, Boston, USA

Crumb rubbers are of interest as a potential source of environmental toxicants due to its widespread commercial use, such as artificial turf which is made from recycled car tires. This is a topic of global concern, as 26,000 artificial turf fields have been installed in the USA and EU to date, with more being installed each year.[1] Tire rubbers contain a complex mixture of chemicals, and people are unknowingly exposed to these potentially toxic compounds when playing on artificial turf fields and playgrounds.[2] While previous studies on crumb rubber focused on well-known contaminants (e.g., metals, PAHs),[2-3] we hope to reevaluate the risk of crumb rubber exposure through identification of unknown compounds.

To accomplish this goal, a non-target analysis (NTA) and quantitative workflow was developed, which utilized the complementary compound coverage from High-Performance Liquid Chromatography-High Resolution Mass Spectrometry (HPLC-HRMS) and Pyrolysis-Gas Chromatography-Mass Spectrometry (Py-GC-MS). Crumb rubber from different artificial turf fields were compared, as well as crumb rubbers at different points of aging. First, novel crumb rubber extraction methods were developed for comprehensive compound identification, in addition to bioavailability-driven extraction methods for exposure analysis and risk assessment. Complementary instrumentation platforms allowed for the identification of unknown organic contaminants and possible transformation products.

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P058

Dissociative Photoionization of Quinoxaline, Quinazoline and Cinnoline

Gülben Sariyar [1], Domenik Schleier [1], Helgi Hrodmarsson [2], Andras Boedi [3], Patrick Hemberger [3], Jordy Bouwman [4]

[1] University of Paderborn, Institute of Technical Thermodynamics, Paderborn, Germany
[2] University of Paris, Laboratory for Astrophysics, Paris, France
[3] University of Paul Scherrer Institute, Laboratory for Synchrotron Radiation and Femtochemistry, Villigen, Switzerland
[4] University of Colorado, Laboratory for Atmospheric and Space Physics, Boulder, USA

Polycyclic aromatic hydrocarbons (PAHs) and their nitrogen-containing counterparts (PANHs) are ubiquitous in extraterrestrial environments ranging from planetary atmospheres to the interstellar medium.[1] After photoexcitation by the interstellar radiation field, they cascade back to the ground state emitting their IR photons on which their presence is based. However, only large PA(N)Hs with more than 50 carbon atoms survive the extreme conditions, whereas smaller ones are destroyed. Their dissociation mechanisms give insights into the cycle of matter in the universe, but so far only singly substituted PANHs have been investigated.[2]

In this work, three nitrogen-containing PANH isomers of $C_8H_6N_2$ composition, quinoxaline, quinazoline and cinnoline, have been studied by dissociative photoionization in a double imaging photoelectron photoion coincidence (i²PEPICO) apparatus at the VUV beamline of the Swiss Light Source. The experimental findings are supported by quantum chemical calculations providing insights into the dissociation mechanism and barriers. To characterize the dissociation kinetics, energy-dependent unimolecular dissociation rates for each channel were calculated as a function of internal energy based on Rice-Ramsperger-Kassel-Marcus (RRKM) statistical rate theory.

The isomers show characteristic dissociation pathways that lead to the elimination of HCN fragments from quinoxaline and quinazoline with barriers of 2.86 and 2.58 eV, respectively. The latter also shows a competing hydrogen loss channel, which occurs not directly at the parent molecule, but instead from the first intermediate on the HCN loss reaction pathway, exhibiting a barrier of 2.56 eV. Even though the H-loss barrier is lower in energy than the HCN loss, the latter is still the main product, which can be explained by a tight transition state leading to a highly constrained hydrogen loss coordinate. In contrast the third isomer, cinnoline, eliminates N_2 instead of HCN, most likely due to the two adjacent nitrogen atoms in its aromatic ring. This route has a barrier of 3.04 eV, which is the highest of all three isomers.

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P059

Chemical Vapour Transport as a Recycling Method for Tellurium from Thermoelectric Materials

Julian Burkhart [1], Lucas Bemfert [1], Eliane Mitura [1], Alexander Sedykh [1], Moritz Maxeiner [1], Ruben Maile [1], Klaus Müller-Buschbaum [1]

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

Tellurium is one of the elements, which could have a supply risk in the future, mainly caused by the high demand for cadmium telluride solar cells.[1] Furthermore, the European import rate of tellurium is close to 100%, because almost the whole tellurium primary production is coupled with Copper and Nickel mining.[1,2] In addition to solar cells, one of the main applications of tellurium-based materials is in thermoelectric devices. Therefore, a suitable recycling method for these secondary resources, namely Bi_2Te_3 and Sb_2Te_3, is necessary. Unfortunately, only a few recycling techniques involving hazardous chemicals or complicated processes are known.[2,3] In 1976 Binnewies published the transport of pure tellurium with sulphur as a transport agent.[4] To use this chemical vapour transport (CVT) as a recycling method, we used sulphur not only as a transport agent but also as an oxidant.[5] In contrast to the existing recycling methods, a simple approach is created without using hazardous chemicals. Tellurium recovery rates exceeding 99% in closed systems with a purity of >99% are possible. Also in open systems, which are more suitable as an industrially usable method, a tellurium purity of >99% was achieved.

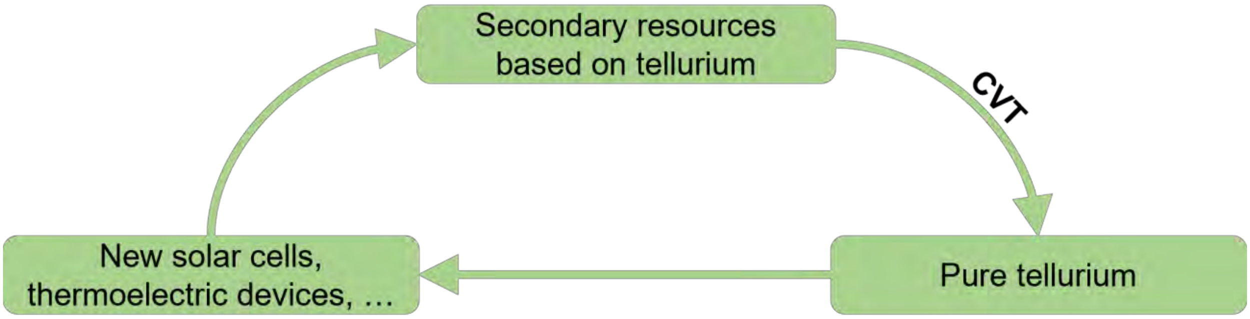

Figure 1: Sustainable life cycle of tellurium using environmentally friendly CVT recycling method.

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P060

Functional Groups Accessibility and the Origin of Photoluminescence in N/O-containing Bottom-up Carbon Nanodots

Paul P. Debes[1], Michal Langer[2], Melanie Pagel[1], Enzo Menna[3], Bernd Smarsly[1], Silvio Osella[2], Jaime Gallego[1], Teresa Gatti[1,4]

[1] Center for Materials Research, Justus-Liebig University, Giessen, Germany
[2] Chemical and Biological Systems Simulation Lab, Centre of New Technologies, University of Warsaw, Warszawa, Poland
[3] Department of Chemical Sciences & INSTM, University of Padua, Padova, Italy
[4] Department of Applied Science and Technology, Politecnico di Torino, Torino, Italy

Due to their exceptional electronic, thermal, optical, chemical, and mechanical properties, 0/1/2D carbon nanostructures (CNSs) have garnered significant interest over the past two decades[1]. Among CNSs, various methods have been developed for synthesizing carbon nanodots (CNDs) from a wide range of small molecules using a bottom-up approach, with numerous applications being explored for these nanomaterials[2,3]. CNDs can be chemically functionalized for sensing, catalysis, and optoelectronic applications, such as investigating light-conversion processes in covalently functionalized CNDs with donor-acceptor organic dyes[4]. This study focuses on characterizing and quantifying the terminal functional groups of four different bottom-up synthesized CNDs[5]. The quantification was achieved through pH back-titrations, Kaiser tests, X-ray photoelectron spectroscopy (XPS), and quantitative ^{19}F-NMR of incorporated fluorine atoms to determine the terminal amine content in the prepared CND samples[6]. The amount of ethylene diamine used as a starting material dictates the fraction of functional groups on the surface. This quantification provides valuable information about the reactivity and accessibility of the terminal functional groups before and after functionalization. By comparing the amounts of terminal amino groups in these four CNDs, it is possible to identify which is most suitable for further functionalization. This allows for determining the theoretical origin of the photophysical properties of the CNDs and comparing them with experimental observations. The study also suggests the presence of polymer-bonded molecular fluorophores (MFs) incorporated into rigid polymer structures as the main contributors to the photoluminescence (PL) properties[7,8].

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P061

yPC meets JCF FJS 2024 in Ulm

Noah Al-Shamery [1]

[1] DBG Deutsche Bunsen-Gesellschaft für physikalische Chemie e.V., Frankfurt am Main, Germany

yPC meets JCF FJS 2024 in Ulm! Early career scientists in Germany benefit from a strong network of chemical societies, which also includes the German Bunsen Society for Physical Chemistry (DBG) and its young Physical Chemists group (yPC). The yPC address questions about the relevance of skills obtained from Physical Chemistry in future careers and the possibility of transitioning outside of your own research field post-Ph.D. – their online events "yPC meets Industry" and "yPC meets Science" are open to all interested early-career researchers.

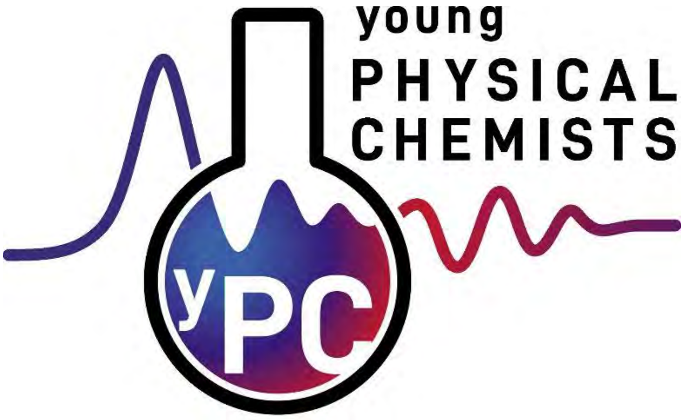

Figure 1: Logo of the young Physical Chemists of the German Bunsen Society for Physical Chemistry.

Additionally, they host a career-focused podium discussion at the annual DBG conference "Bunsen-Tagung" and a networking evening for young society members (www.bunsentagung.de), frequently in collaboration with the local German Young Chemists' Network. The yPC award the Agnes Pockels Prize for the best PhD thesis in Physical Chemistry, which is open to researchers all across Europe. Furthermore, the yPC act as annual guest editors for the DBG's *Bunsen-Magazin*, providing a platform for young researchers to discuss important topics and amplify their voices in the society, and assist the *Nachrichten aus der Chemie* in the selection of authors for the *Trendberichte Physikalische Chemie*. If your interest in our activities has been piqued, feel free to come by our poster and learn how you can become part of our society as well. We look forward to seeing you!

P062

Direct Imaging of Electrochemical Palladium Hydride Formation from $PdCoO_2$ for Highly Efficient Hydrogen Evolution Reaction

Se-Ho Kim[1,2] , Luca Camuti[3,4], Filip Podjaski[3,5], Andrea M. Mingers[1], Tolga Acartürk[3], Ulrich Starke[3], Bettina Lotsch[3,4], Christina Scheu[1], Baptiste Gault[1,6], Siyuan Zhang[1]

[1] Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
[2] Korea University, Department of Materials and Engineering, Republic of Korea
[3] Max-Planck-Institute for Solid State Research, Stuttgart, Germany
[4] Ludwig-Maximilians-Universität, Department of Chemistry, Munich, Germany
[5] Imperial College, Department of Chemistry, London, United Kingdom
[6] Imperial College, Department of Materials, Royal School of Mines, London, United Kingdom

Active and reliable electrocatalysts are fundamental to renewable energy technologies.[1] PdCoO2 has recently been recognized as a promising catalyst for the hydrogen evolution reaction (HER) in acidic media.[2] In this poster, the activation process of the catalyst is revealed, which involves leaching out of Co atoms from the template as well as the formation of palladium hydride nanoparticles. The former process is studied by operando measurement of Co dissolution and found to be kinetically related to HER. The as-formed hydride nanoparticles were found to be stable up to anodic potentials of 0.8 V (with respect to reversible hydrogen electrode at pH = 1).

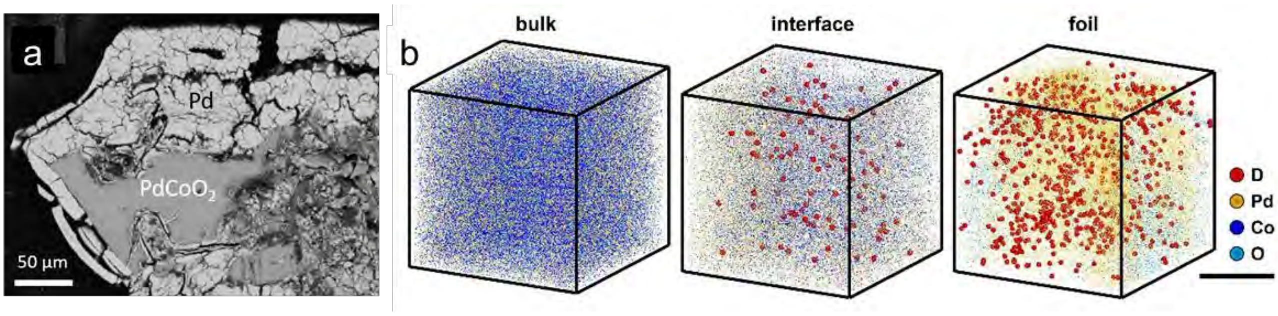

Figure 1: a) As-formed PdH_x capping layer formed on top of a 140 h aged PdCoO2 crystal. b) Reconstructed 3D atom maps of the bulk, interface, and Pd-rich capping regions. The scale bar is 10 nm.

The latter, i.e. the formation of hydrides, is confirmed through secondary ion mass spectrometry and quantitatively analyzed by atom probe tomography. Here, deuterium was employed as the hydrogen indicator, resulting in the determination of the PdD_x phase and a calculated D/Pd atomic ratio of 0.28.

We showcased the high HER activity and stability of Pd hydride nanoparticles derived from PdCoO2 particles.

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P063

Investigation of The Effects of Carbon Anode Precursors on Electrochemical Performance in Na-ion Batteries

Şebnem Cingisiz [1], İrem G lersönmez [1], Edanur Aktürk [1], Rezan Demir-Cakan [1]

[1] *Gebze Technical University, Department of Chemical Engineering, Kocaeli, Turkey*

In the search for alternative batteries, sodium-ion batteries (NIBs) are promising because they provide low cost, sustainable and safe raw material sources. Graphite, which is used as the anode in almost all commercial LIBs, has a very crystalline structure, and the distance of 0.335 nm between the graphene layers does not allow the intercalation of Na^+ ion with conventional carbonate based electrolyte.[1] Many different anode materials are being developed as an alternative to graphite. Among these, irregular structured carbons are used as anode materials in almost all NIB prototype batteries. Biomass or petroleum waste sources, which are generally low-cost, are used as carbon precursors. These carbons include both soft carbon (SC) and hard carbon (HC) structures.[2,3]

In this study, the performances of biomass-derived HC and petroleum waste-derived SC materials as anodes in SIBs were investigated. Preliminary results showed that both SC and HC electrodes exhibit stable performance, but the HC anode provides higher capacity at a current density of C/10 in carbonate electrolytes. The influence of carbon sources and electrolyte solvents will be discussed during the presentation.

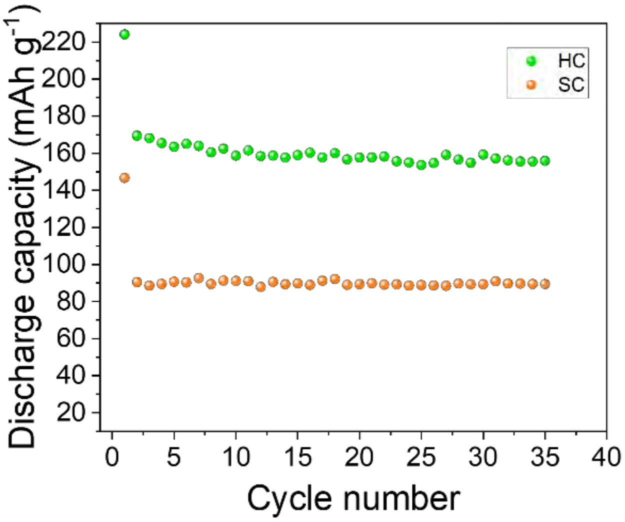

Figure 1: Cycle performances of HC and SC anodes at a current density of C/10 (1C=372 mA g^{-1}).

Acknowledgement

The authors appreciate the financial support from TUBITAK (123M536).

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P064

Synthesis and characterization of a pyrene-4,5,9,10-tetraone substituted conductive polyaniline polymer.

Nazmiye KILIÇ[1], Yasemin SOLMAZ[1], Merve GÜNER[1], Rezan DEMİR-ÇAKAN[2,3], Serkan YEŞİLOT[1]

[1] *Gebze Technical University, Department of Chemistry, Kocaeli, Turkey*
[2] *Gebze Technical University, Department of Chemical Engineering, Kocaeli, Turkey*
[3] *Gebze Technical University, Institute of Nanotechnology, Kocaeli, Turkey*

The development of redox-active, high-performance conductive materials is important for energy storage systems.[1] In this respect, organic carbonyl compounds are promising groups for electrode materials due to their lightweight, molecular variety, and stability in redox reactions. In particular, the pyrene-4,5,9,10-tetraone structure stands out because it contains four carbonyl functional groups as electrochemical active sites.[2] Conductive polyaniline (PANI) polymer, another special group for energy storage systems, has unique redox properties, good conductivity, low cost, and ease of synthesis. Polyaniline structures can be synthesized with different monomer types using chemical methods.[3] Thus, the electrochemical properties can be varied with polyaniline polymers obtained from modified monomers. In this way, it is possible to obtain remarkable materials for energy storage applications.

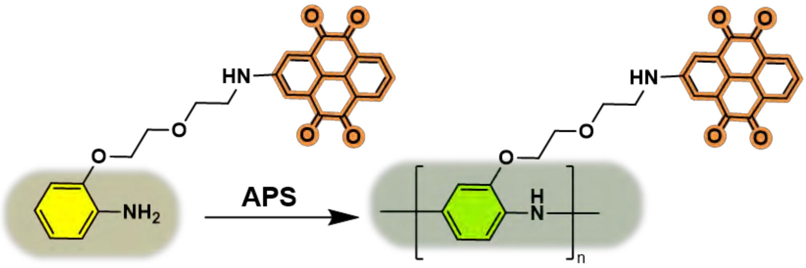

Figure 1: Synthetic pathway of pyrene-4,5,9,10-tetraone substituted polyaniline.

In this work, conductive polyaniline polymer was synthesized using aniline monomer substituted by pyrene-4,5,9,10-tetraone (Figure 1) and characterized using appropriate standard spectroscopic methods. The thermal (DSC and TGA), surface (SEM), and electrical conductivity properties of this polymer were examined. Additionally, the optimized structure of the polymer was investigated using the DFT method.

We wish to thank the GTU-ADEP (2023-A-113-13) Project for their support and TUBITAK ULAKBIM, High Performance and Grid Computing Center (TR-Grid e-Infrastructure) for calculations.

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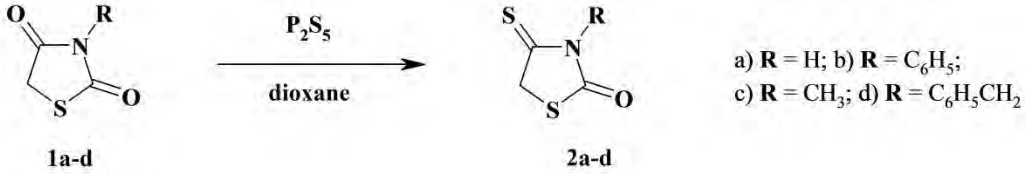
P065

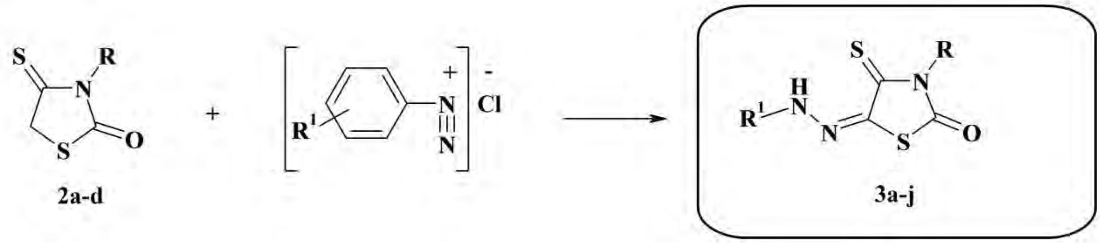
Antioxidant properties of some 4-thioxo-thiazolidin-2-ones

Viktoria A. Lozynska [1], Zoriana I. Chulovska [1], Taras I. Chaban [1], Olena. V. Klenina [1], Iryna V. Drapak [1], Ihor G. Chaban[1], Volodymyr V. Ogurtsov [1]

[1] Danylo Halytsky Lviv National Medical University, Lviv, Ukraine

Thiazolidinone derivatives are a traditionally known class of biologically active compounds. The results of recent studies of the chemistry and biological activity of the specified class of connections convincingly showed that they are promising as pharmacological agents with a broad spectrum of activity. As a continuation of our research work in reference to the design of new biologically active azaheterocycles, in this work we reported about of synthesis, anticancer and antioxidant activities of 4-thioxo-thiazolidin-2-ones. The corresponding thiazolidine-2,4-diones (**1**) obtained by the known method was introduced into the thionation reaction with phosphorus pentasulphfide, which led to yielding the interesting in chemical and biological terms 4-thioxo-thiazolidine-2-ones (**2**). The active methylene group presence in C^5 position provides an entry for its utilization in azo coupling reaction with aryldiazonium salts. It was found that compounds 2a-d reacts with salts of aryldiazonium leading to appropriate 5-arylhydrazo derivatives of 4-thioxo-thiazolidin-2-one **3** generation.





The antioxidant activity was determined on the basis of free radical scavenging activity of stable 2,2-diphenyl-1-picrylhydrazyl (DPPH). The effect of the studied compounds on DPPH radicals was estimated according to the method of Blois with minor modifications. Ascorbic acid was used as a standard. Percentage of free-radical-scavenging activity was expressed as percent inhibition. The antioxidant activity evaluation results showed that, in general, most of the tested compounds possess insignificant free radical scavenging effect being in the range of 7.15%- 12.50%. However, when compared with existing antioxidants, some our compounds were found to be more potent.

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P066

UHV-studies of adsorbed CO_2 on Cu and Cu_2O at Rutile (110)

Justin Klimek [1], Maximilian Grebien [1], Katharina Al-Shamery [1]

[1] University of Oldenburg, Institute of Chemistry, Oldenburg, Germany

Carbon dioxide (CO_2) is one of the major greenhouse gases causing the worldwide climate change thus making it desirable to recycle carbon dioxide as a contribution to remove anthropogenic produced CO_2.[1] Therefore it is desirable to capture and use anthropogenic CO_2 as an organic feedstock for various products like methanol, which is already synthesized from H_2 and CO_2 (syngas) using a $Cu/ZnO/Al_2O_3$ catalyst. But studies have shown that the use of CO_2 affords lower yields than the use of CO, thus, showing the need for the development and investigation of new, more efficient catalysts.[2]

Interesting systems are mixed oxides such as TiO_2/WO_3 [3] as well as Au or Cu on TiO_2 which have shown high reactivity towards methanol reactions due to Ti^{3+} as reactive center for interaction with oxygen.[4] Literature has also shown that formation of methanol from syngas using Cu-based nanocatalysts is possible.[5]

In this work we present the preparation of nanoparticulate copper and cuprous oxide on Rutile (110) of different reduction degrees, prepared via electron beam evaporation under UHV conditions and high-pressure oxidation in a chamber connected to the UHV-system. These systems were characterized with X-ray photoelectron spectroscopy (XPS) and the reaction behaviour of CO_2 and coadsorbates was investigated with temperature programmed desorption spectroscopy (TPD). The performed experiments show cluster-size-dependent formation of carbon monoxide and CO_2-coverage-dependent adsorption-site-sensitive desorption of CO_2.

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P067

Photocatalytic Properties of Zn(II) Coordination Polymer Constructed From a Cyclotriphosphazene-Functionalized Ligand and Terpyridine

Yunus Zorlu [1*], Elif Özcan [1], Ayşe Nur Kartal [1]

[1] *Gebze Technical University, Department of Chemistry, 41400 Kocaeli, Türkiye*

Growing concerns about water pollution from organic dyestuff pollutants due to technological advancements and urban/industrial growth have fueled demand for rapid and accurate measurement methods. Despite approaches like adsorption and membrane separation, challenges such as cost and low efficiency persist, underscoring the need for highly efficient and environmentally friendly methods. Photocatalysis, with its advantages in water remediation, pollutant removal, H_2 production, and CO_2 conversion, emerges as a promising solution for sustainable environmental practices.[1] Coordination polymers, formed through coordination bonds between metal ions and organic ligands, exhibit versatile functional order in porous structures, finding applications in energy storage, catalysis, and gas adsorption.[2]

This research evaluates the potential of newly synthesized Zn(II) cyclotriphosphazene-based coordination polymer, **Zn(II) PCP**, as a photocatalyst for wastewater treatment. **Zn(II) PCP** was obtained by employing a cyclotriphosphazene ligand functionalized with tetracarboxylic acid and N-donor ligand (terpyridine), and then precisely characterized using techniques such as single-crystal XRD, PXRD, TGA, FTIR, SEM-EDX, and UV-DRS measurements. The photocatalytic efficiency of **Zn(II) PCP** is then explored for specific dye removal methylene blue, methyl orange, and rhodamine B, highlighting its promise for environmental and industrial photocatalysis. Overall, this study contributes valuable insights to the development of efficient and sustainable photocatalytic materials.

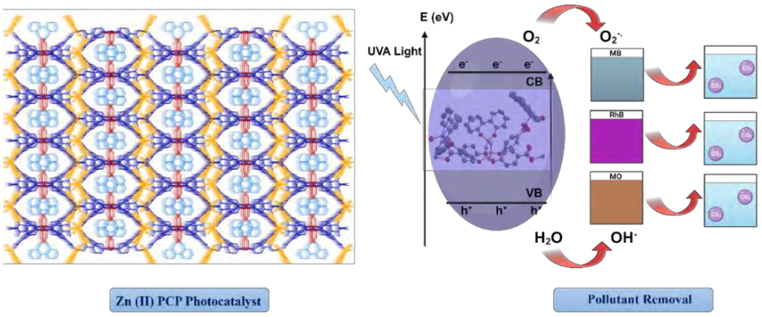

Figure 1. The photocatalytic degradation of water contaminants through the application of Zn(II) PCP photocatalyst under UVA light exposure.

The authors would like to acknowledge the financial support of the TUBITAK-122Z456

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P068

Characterization of Sm^{3+}-Activated Carbonated Calcium Chlorapatite Phosphors for Theranostic Applications: A Comparative Study of Co-precipitation and Hydrothermal Methods

Katarzyna Szyszka [1] and Rafal J. Wiglusz [1,2]

[1] Institute of Low Temperature and Structure Research, PAS, Okolna 2, PL-50-422 Wroclaw, Poland

[2] Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, Faculty of Chemistry, Silesian University of Technology, Krzywoustego 4, 44100 Gliwice, Poland

Continuous efforts are ongoing to discover new luminescent materials with appropriate properties for applications in medicine, serving as theranostic agents for healing and bioimaging [1–3]. The novel single-phase carbonated calcium chlorapatite ($Ca_{10}(PO_4)_5(CO_3)Cl_2$, abbreviated as CaClAp-$CO_3$) phosphors activated with varying concentrations of Sm^{3+}ions were successfully fabricated using both co-precipitation and a hydrothermal methods to investigate the influence of the synthesis techniques on the physicochemical properties of these materials. The effects of doping concentration of Sm^{3+} ions and synthesis technique on the structure, photoluminescence (PL), energy transfer, substitute site, fluoresce lifetime and luminescence colour of phosphor were investigated.

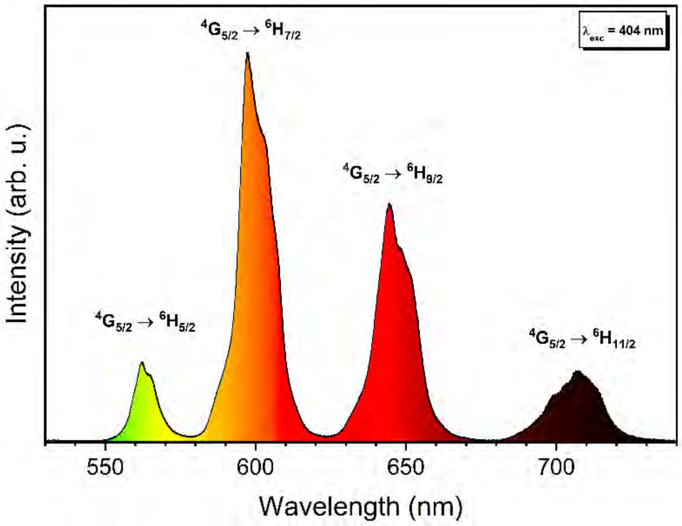

Figure 1: Emission spectrum of the Sm^{3+}-doped $Ca_{10}(PO_4)_5(CO_3)Cl_2$ prepared via hydrothermal synthesis.

All obtained materials emit reddish-orange light with the most intense transition of $^4G_{5/2} \rightarrow {}^6H_{7/2}$. The ED/MD ratio, CIE colour coordinates and colour purity were determined to provide additional insights into the spectroscopic attributes of the obtained phosphors. In addition, the concentration quenching was also observed, and its mechanism was proposed based on theoretical calculation showing the multipolar interactions.

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P069

The physical organic chemistry underlying mucin function

Carolyn Barnes [1], Jill Alty [1], Austin G. Kruger [1], Dayanne Carvalho [1], Spencer D. Brucks [2], Laura L. Kiessling [1]

[1] Massachusetts Institute of Technology, Department of Chemistry, Cambridge, United States
[2] Harvey Mudd College, Department of Chemistry, Claremont, United States

All animals possess a crucial mucus layer over their epithelial cells, which serves as a first line of defense against environmental threats. The primary constituents of mucus are elongated, densely *O*-glycosylated proteins called mucins. The elongated and rigid structure of mucins is unique and known to play an important role in many of mucins' native functions. While glycosylation and backbone stereochemistry have been investigated for their impact of mucin structure and function, the contributions of other factors, such as charge and polymer architecture, have not been thoroughly explored. Native mucins hold promise as innovative antibacterial and protective materials; however, their isolation remains challenging, impeding both biological understanding and accessibility. Studies of the structure–function relationships of these materials could expedite their use and lead to synthetic mucins with beneficial applications. Thus, we generated defined, synthetic mucin analogs to identify the key structural characteristics that govern mucin function. Previous studies from our group showed the critical role of an extended backbone for mucin-mimetic polymers.[1] In this study, we use polynorbornene (PNB) mucin mimics to explore how different mucin features contribute to their structure. We varied backbone stereochemistry by exploiting ring-opening metathesis catalysts that give rise to backbones with either cis or trans alkenes. As many of the glycans that mucins bear are charged, we examined how appending negatively charged glycans influences mucin mimic architecture. To impart brush-like architectures, we examined the consequence of changing the glycan linker length. This presentation will focus on how these different features influence synthetic mucin architecture and, by extension, the observed conformations in native mucins. We expect that elucidation of the molecular underpinnings of mucins' physical properties will guide the development of improved mucin-mimetic therapeutics.

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Developing Redox Active Species and Cell Design for Redox Flow Batteries.

Karin Sowa [1], Prof. Martin Winter [2], Mariano Grünebaum [2]*

[1] Westfälische Wilhelms-Universität Münster, Baccara, 48149 Münster
[2] Forschungszentrum Jülich GmbH, Helmholtz Institute Münster, IEK-12, Correnstraße 46, 48149 Münster, Germany

Energy Grid storage has evolved into a key technology for improving sustainability in the power generation sector[1], and redox flow batteries (RFBs) are promising for this application. Unlike common batteries, RFBs work with soluble redox-active species dissolved in liquid electrolytes and stored in large tanks. The electrolyte is pumped through an electrochemical reactor in which the active species are oxidised or reduced. The size of the reactor determines the rated power, while the tank volume determines the total energy capacity, which allows for a unique scalability of this architecture.[2]

To date, the vast majority of RFB literature reports have focused on aqueous electrolytes, arguably due to the success of the commercially available vanadium RFB. However, the disadvantage of aqueous electrolytes is the relatively small electrochemical window (ESW).[3]

Non-aqueous RFBs (NAqRFBs) not only offer a larger ESW but can also be combined with organic redox-active species instead of metals such as vanadium. The gradual substitution to organic materials could reduce costs and transport, simplify disposal and enable more flexible adjustment of the redox potential using synthetic methods for modifications. So far, however, there are no NAqRFBs that match or even exceed the performance of aqueous RFBs. Challenges investigated are the limited solubility of active species and their cross over at the membrane. In addition, cell design, flow cell technology and the choice of material for the electrodes and separator have a major impact on the overall performance of the RFB cells and are tested and evaluated.[4]

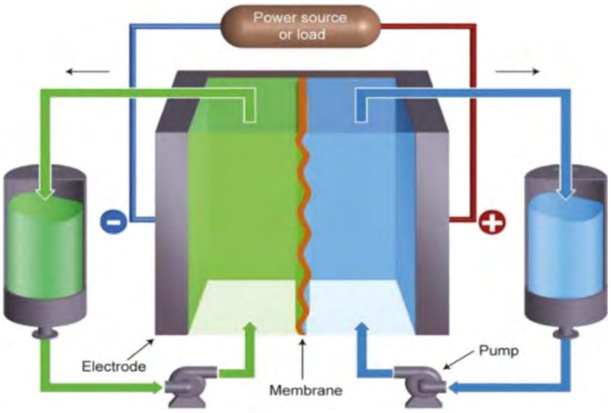

Figure 1: Exemplary Redox Flow Battery

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P071

Functionalization of Polymer Particles for Chromatography Applications via Atom Transfer Radical Polymerization and Click Chemistry

Luca Schipplick [1], Andreas Seubert [1]

[1] *Philipps University Marburg, Department of Chemistry, Marburg, Germany*

Polymer based stationary phases are the most common materials for ion chromatography. Since the application of ion chromatography extended to more complex organic analytes, it is necessary to develop stationary phases with enhanced selectivities. This requires new functionalization methods for polymer particles.[1]

One approach is the direct functionalization of porous polystyrene divinylbenzene (PS/DVB) particles with heterogenous atom transfer radical polymerization (ATRP). For heterogenous ATRP an initiator is linked to the polymer particle followed by a solid phase polymerization of functional monomers. The unequal accessibility of initiator molecules on the surface leads to an inhomogeneous functionalization.[2]

Goal of this work is to develop a synthetic route for a more homogeneous functionalization of polymer particles. With the application of homogenous ATRP in solution, followed by a click reaction between the macromolecule and the particle surface, a more homogeneous distribution of the functionalization is achieved. This also permits an easier characterisation of the low molecular weight functionalities just before the click step.

At first, ATRP is used to synthesize macromolecular chains of styrene sulfonic acid, styrene phosphonic acid and styrene carboxylic acid. To characterize the chain length and uniformity, NMR spectroscopy and size exclusion chromatography are used. Starting from a polymerization initiator with an alkyne functionality, alkyne-azide click chemistry can be used to functionalize PS/DVB particles with the polymer chains. Chromatographic cation retention is used as indicator for the degree of functionalization.

This approach allows the homogenous functionalization of PS/DVB particles with various functional groups.

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P072

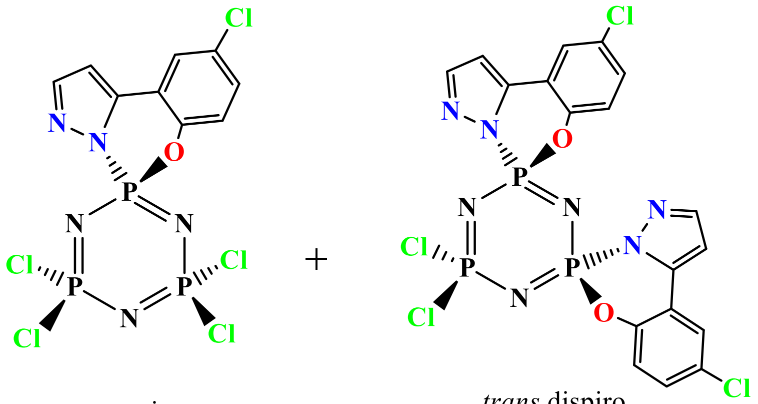
Chloro phenol pyrazole appended cyclotriphosphazene compounds: Synthesis and characterization

Esma MUTLU [1], Duygu PALABIYIK [1], Ceylan MUTLU BALCI [1], Serap BEŞLİ [1]

[1] *Gebze Technical University, Faculty of Basic Science, Kocaeli, TURKEY*

Cyclotriphosphazenes, which are in a class of inorganic ring compounds, can undergo nucleophilic substitution reactions thanks to their active phosphorus halogen bonds, and as a result of these reactions, new types of inorganic-organic hybrid molecules can be synthesized easily and efficiently.[1,2] Pyrazole derivatives are the most studied compounds in pharmaceutical chemistry because they have a wide variety of biological activities such as antimicrobial, anti-fungal, anti-tuberculosis, anti-inflammatory, anti-cancer, anti-viral and neuroprotective.[3] In this study, new types of inorganic-organic hybrid molecules that are expected to show potential biological activity were synthesized.

In here, the reactions of hexachlorocyclotriphosphazatriene (trimer) (**1**) and 4-chloro-2-(1H-Pyrazol-3-yl)phenol (**2**) were carried out in the presence of NaH base at different molar ratios. As a result of the necessary separation and purification processes, mono spiro (**3**), trans dispiro (**4**) were obtained. The structures of the obtained products were clarified by ^{31}P and ^{1}H NMR spectra, mass, and element analysis results and compounds **3** and **4** crystal structures were determined by the single X-Ray diffraction method.



mono spiro **(3)**

trans dispiro **(4)**

Figure 1: The reaction of hexacyclotriphosphazene (1) with 4-chloro-2-(1H-pyrazol-3-yl)phenol (2).

The authors would like to thank the Scientific Research Projects (BAP) coordination of Gebze Technical University for financial support (grant 2023- A-105-17).

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P073

Career Network and Outreach Efforts for Younger Chemists

Owen Grimm[1,2]

[1] Northeastern Section Younger Chemists Committee, Boston, USA
[2] DuPont, Marlborough, Massachusetts, USA

The mission of the Northeastern Section American Chemical Society (NESACS) Younger Chemists Committee (YCC) is to advocate and facilitate the professional development of young chemists in the Greater Boston Area and to cultivate future leaders in chemistry. We are predominantly a community of undergraduate students, graduate students, and young professionals in the greater Boston, USA area.

Frequently students graduate without a clear idea of what they want to do with their degree. We endeavor to provide younger chemists with the insight and connections to start their careers through our events and by working with universities to encourage students to become more active with the local ACS section. YCC offers career insights with our events showcasing different career options in chemistry. Partnering with the NESACS Senior chemists committee and local universities, invited speakers from various career paths share their insights on career paths to student attendees. Additionally, YCC hosts an annual research conference which provides an opportunity for local undergraduate students, graduate students, postdoctoral fellows, and early-career scientists to present their research to their peers. It is also an opportunity for presenters to network with professors and industry professionals from the Boston area.

Figure 1: Career Luncheon at 2024 Northeast Region ACS meeting

To further interface this growing body of younger chemists with the larger chemist community, new formats are being explored for NESACS monthly meetings, including panel discussions and networking receptions, which have been popular with the younger community.

P074

Towards the Synthesis of 2-Dithiophene-tetrazole-5-*meta*[6]Cycloparaphenylene for Imaging Applications

Johannes Voigt [1], Hermann A. Wegner [1]

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

Fluorescence imaging is crucial for targeting specific cellular molecules like proteins, using different labelling methods such as the tetrazole photoclick reaction.[1,2] Small organic molecules, as a class of fluorophores are favoured for their brightness, photostability, and colour range but also come with limitations.[1,3] Notably, cycloparaphenylenes (CPPs) have emerged as a novel scaffold for fluorophore dyes over the last two decades.[4,5]

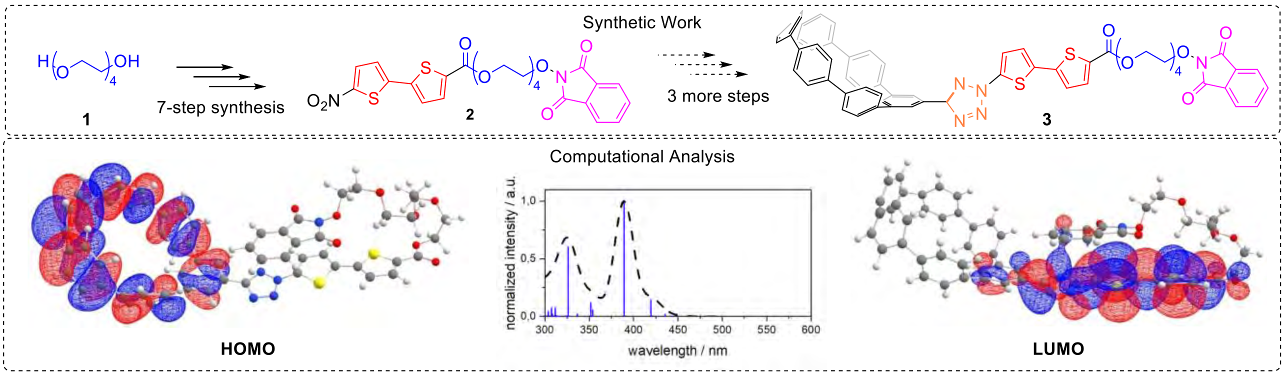

Figure 1: Graphical Abstract showing the synthetic work (top) as well as HOMO and LUMO of the 2,5-diaryl tetrazole (bottom, left and right) and a predicted UV-Vis spectrum of this compound (bottom, middle).

Inspired by these previous achievements, we chose a modular synthesis approach for a new 2,5-diaryl-tetrazole (**3**). We developed a seven-step synthesis route leading to a precursor **2**. Complementing our synthetic, we conducted computational analyses to explore the photophysical properties of the envisioned 2,5-diaryl tetrazole.[6] Our next objective would be to complete the synthesis with introducing the *m*[6]CPP moity and perform UV-Vis measurements and compare those results with the computational predictions.

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P075

Better understanding of selective transformation of Si–N,O-functionalized organosilanes

Jan-Lukas Kirchhoff [1], Michael Nuss [1], Tristan Mairath [1], Carsten Strohmann [1]

[1] *TU Dortmund University, Faculty of Chemistry and Chemical Biology, Dortmund, Germany.*

Aminoalkoxyorganosilanes represent suitable reactive intermediates in silicon chemistry that offer high potential for the selective synthesis of silicon surfaces and two- as well as three-dimensional silicone networks.[1,2] This helps to achieve a better understanding of transformations in principle and can precisely control these transformations.[3,4]

In this research, the electronic structure obtained from high resolution single-crystal X-ray structure analysis, spectroscopic investigations and DFT calculations are used to determine which reagents lead to the selective cleavage of alkoxy or amine groups at the silicon center.

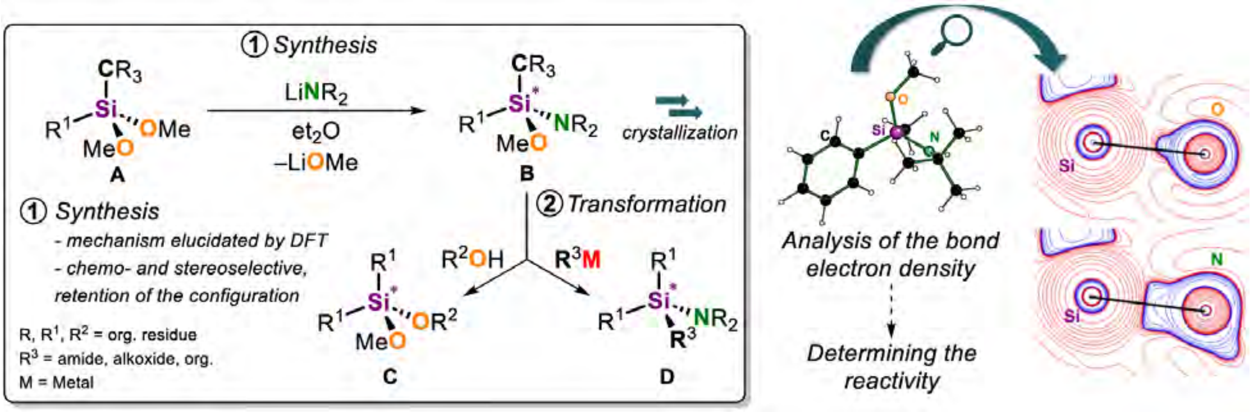

Figure 1: Reactivity studies of aminomethoxysilanes: Selective differentiation of the respective functional groups

As part of the investigations, various aminomethoxysilanes were first synthesized chemoselectively, chiral compounds were even synthesized stereochemical pure. Subsequent transformations for the selective cleavage of Si–N- and Si–O-bonds confirmed that particularly strong nucleophiles, such as metal organometals, substitute methoxy groups at the silicon center. In contrast, the presence of alcohols leads to a selective cleavage of the Si–N-functionality. High-resolution single-crystal X-ray structure analysis of aminomethoxysilanes shows that the bond electron densities differ significantly, which has a direct influence on the reaction mechanisms. This technique offers a precise as well as transferable tool for reactivity predictions in research.

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P076

An Unsymmetrical Diborane(4) as a Facile Precursor to PBP Boryl Pincer Complexes

Philipp Rutz [1], Jörg Grunenberg [2], Christian Kleeberg [1]

[1] *Technische Universität Braunschweig, Institut für Anorganische und Analytische Chemie, Braunschweig, Germany*

[2] *Technische Universität Braunschweig, Institut für Organische Chemie, Braunschweig, Germany*

The synthesis of PBP aminoboryl pincer complexes introduced in 2009 by Yamashita and Nozaki et al. Has thus far been restricted to B-H oxidative addition of Diaminoborane ligand precursors to transition metal precursors.[1] This limitation has hindered the field's progress. Consequently, we developed a new process to access PBP boryl pincer complexes via an unsymmetrical diborane(4), a class of compounds established as boryl ligand precursors.[2] The unsymmetrical diborane(4), d(CH$_2$P(*i*Pr)$_2$)abB–Bpin (pin = (OCMe$_2$)$_2$; d(R)ab = 1,2-(RN)$_2$(C$_6$H$_4$)), was obtained by reacting a copper(I) boryl complex (boron nucleophile) with a boron electrophile, the borane d(CH$_2$P(*i*Pr)$_2$)abB–H; a protocol we established as a general route to unsymmetrical diborane(4) derivatives.[3] This diborane(4) precursor can be used as a precursor to prepare PBP boryl pincer complexes. The versatility of this method was demonstrated by preparing copper and platinum complexes, [(d(CH$_2$P(*i*Pr)$_2$)abB)Cu]$_2$ and *trans*-[(d(CH$_2$P(*i*Pr)$_2$)abB)Pt–Bpin], as well as a series of group nine boryl complexes with the general formula (d(CH$_2$P(*i*Pr)$_2$)abB)M(PMe$_3$)n (n = 1, 2).[4,5]

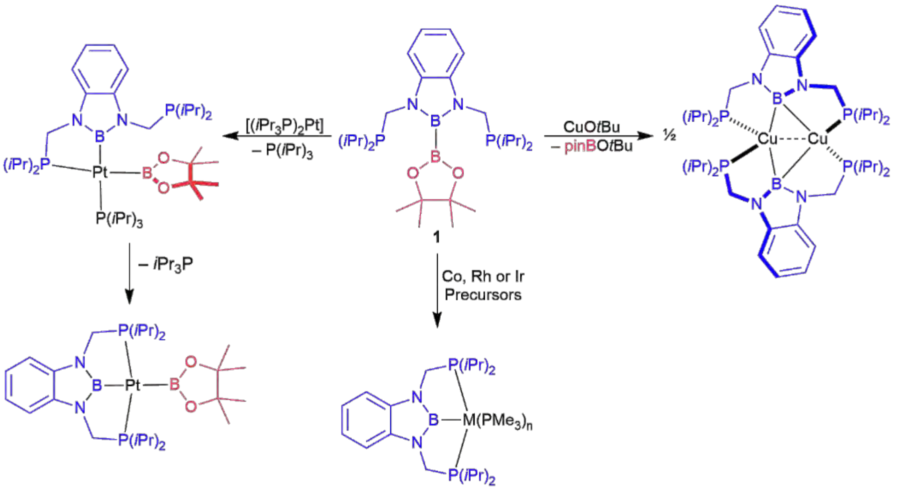

Figure 1: Reactions of d(CH$_2$P(*i*Pr)$_2$)abB–Bpin with transition metal precursors.

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P077

PHOTOREACTIVITY OF 2-AZIDOIMIDAZOPYRIDINES MONITORED BY ^{19}F-NMR SPECTROSCOPY

Corinna von Schmuda Trzebiatowski and Thomas Lindel

TU Braunschweig, Institute of Organic Chemistry, Braunschweig, Germany

The chemistry of photoreactive analogues of DNA and RNA bases continues to be of broad interest. In the field of photoaffinity labelling, azidopurines have received considerable attention.[1] After losing dinitrogen, nucleophilic attack by various nucleophiles has been observed including by those present in biochemical binding partners.[2] The reactions did not always lead to a single product, which raises the question how nitrogen-deprived analogues would behave. To our knowledge, the photochemistry of 8-azidodeazapurines has not been studied in detail, whereas there are several studies on 8-azidopurines. Deazapurines occur as building blocks of biologically active agents.[3] They are also valuable for studying the chemistry of DNA and RNA itself.[4] Our work on the chemistry 2-azidobenzimidazoles (bis-deazapurines)[5] encouraged us to investigate the synthesis and photoreactivity of 1- or 3-deazaazidopurines, which is subject of this communication.

We synthesized a series of new 1- or 3-deazaazidopurines starting from pyridine-derived building blocks. We installed fluorinated functionalities that enabled facile monitoring of irradiation product mixtures by ^{19}F NMR. The compounds were subjected to irradiation in both flow and flask setups, both in the absence and the presence of potential reaction partners.

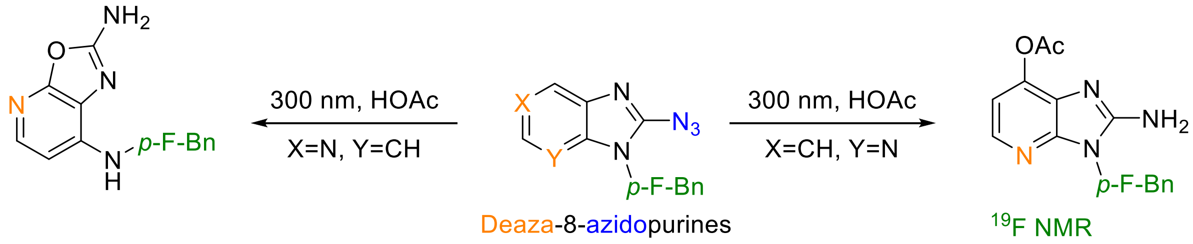

Figure 1: Example of irradiation experiment of two 2-azidoimidazopyridines in the presence of acetic acid.

Irradiation products revealed to be dependent on the position of the nitrogen in the pyridine section and on the setup of the irradiation experiment (flask *vs.* flow). For instance, we obtained an unexpected oxazolo[5,4-*b*]pyridine, the structure of which was analysed for the existence of isomers employing the WebCocon tool.

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P078

NOVEL HEXACARBOXYLATE LIGAND for Zr-MOF SYNTHESIS

B. Topaloğlu Aksoy [1], B. Çoşut [1]

[1] Gebze Technical University, Department of Chemistry, Kocaeli, 41400 TURKEY

One of the most important porous material classes that has been studied frequently in recent years is metal-organic frameworks that is called as MOFs. They are crystalline semiconductor like porous materials which are a class of coordination polymers [1]. To form the framework structure, building blocks are linked with co-ordination covalent bonds. There are more than organic ligand types to construct rigid or flexible MOF structures. Due to the different coordination shapes of carboxylate groups, multicarboxylate ligands are one of the important ligand types for the design of MOFs. To construct a MOF structure formed by multicarboxylate ligand, cyclotriphosphazene core is an ideal platform [2]. The cyclotriphosphazene core consists of six arms at the periphery and a nitrogen-phosphorus ring as core and it is known as inorganic scaffold [3]. By using cyclotriphosphazene core with different carboxylate groups, various flexible multicarboxylate ligands for the design of MOFs can be prepared. The primary objective of this study is to fabricate new multicarboxylate ligand based on cyclotriphosphazene for the construction of novel Zr-MOFs.

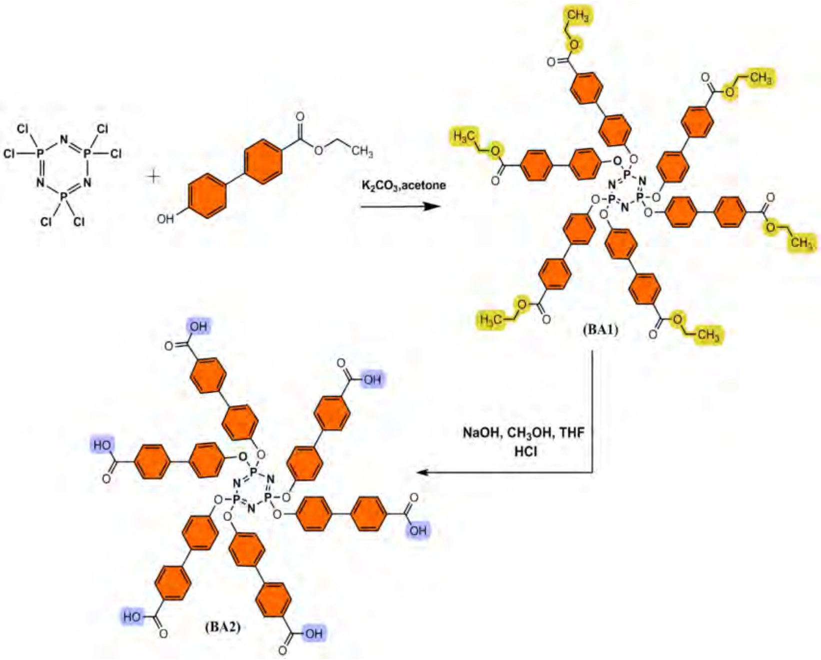

Figure 1: Synthesis outline of the cyclotriphosphazene derived hexacarboxylate ligand

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P079

Retention behaviour of per- and polyfluoroalkyl substances (PFAS) on anion exchangers

Jumana Khoury [1], Andreas Seubert [1]

[1] *Philipps University Marburg, Department of Chemistry, Marburg, Germany*

Per- and polyfluoroalkyl substances (PFAS) are widely used for industrial and commercial applications, such as food packaging and household articles. Their global environmental distribution has grown since the 1950s, resulting in a worldwide contamination of PFAS in soils, surface and groundwater. Due to their persistent, bioaccumulative and partially toxic properties, the development of analytical methods with high selectivity and sensitivity has become crucial.[1]

PFAS analysis is commonly performed by using liquid chromatography mass spectrometry methods. Long chain PFAS (C ≥ 8) can be separated with reversed phase columns based on their hydrophobic properties. For the separation of volatile and semi-volatile PFAS, gas chromatography can be applied. Many representatives of PFAS contain ionic functional groups. While there exist several studies on PFAS removal by ion exchange resins, ion exchange chromatography has barely been used for their separation. Apart from ionic interactions, ion exchangers offer hydrophobic and hydrophilic retention mechanisms, which is why ion chromatography might be a suitable application with unique separation selectivities.[2–4]

The aim of this study is to characterize retention behaviour of PFAS on multiple anion exchange columns. Therefore, the influence of system parameters like pH, organic modifier and column temperature on analyte selectivity is investigated.

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P080

Design of templated porous structures with atomic layer deposition

Júlio C. S. Terra, Jeremy S. Luterbacher

École Polytecnique Fédérale de Lausanne, Laboratory of Sustainable and Catalytic Processing (LPDC), Lausanne, Switzerland

Heterogeneous catalysts are omnipresent in the petrochemical industry and have inherent advantages in product purification and recyclability. They will likely play an important role in the transition to a more renewable and circular chemical industry. The difficulty in controlling their active sites and architectures, however, is a drawback[1] , especially for feedstocks that are rich in chemical functionality (*e.g.* biomass).[2]

Atomic layer deposition (ALD) is traditionally a vapour-phase technique used to coat surfaces with atomic precision;[3] it relies on an excess of reactants that need to be purged after each coating cycle, making the method incompatible with pore-generating techniques such as soft templating (*i.e.* when self-assembling structures are used to direct the synthesis of solid materials and then removed by calcination or solvent extraction).[4] Some of these issues can be overcome by liquid-phase ALD, a technique that was developed by the Luterbacher group.[5] It consists of titrating the surfaces to determine the exact number of available reaction sites, so stoichiometric amounts of reactants are added to the solution instead of excesses, avoiding the purging step and making it a versatile approach to ALD.

Therefore, we take advantage of the combination of the chemical composition control provided by ALD with the morphology control provided by structure-directing templates, creating a powerful tool to be explored using liquid-phase ALD (Figure 1). This technique notably provides a unique opportunity for manufacturing highly tuneable heterogeneous catalysts to be employed in complex chemical transformations.

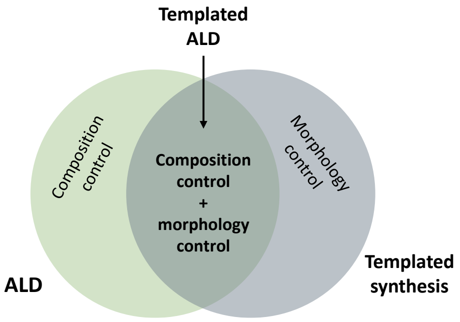

Figure 1. Combination of the advantages of ALD and templated synthesis in templated ALD: high control on both composition and morphology of the resulting nanomaterial.

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P081

Enantioselective Suzuki-Miyaura Cross-Coupling of *meso* Bis(boronic) Esters

Paul S. Lee [1], Mingkai Zhang [1], Bill Eugene [1], Christopher Allais [2], Robert A. Singer [2], James P. Morken [1]

[1] Boston College, Department of Chemistry, Chestnut Hill, MA USA
[2] Pfizer Worldwide Research and Development, Groton, CT USA

The Suzuki-Miyaura cross-coupling reaction has remained a powerful tool for synthetic chemists to forge C–C bonds, particular between C(sp^2) partners, and is often air and moisture tolerant at low catalytic loadings.[1] The prevalence of stereocentres in pharmacological compounds has led to a burgeoning interest in the asymmetric transformation of C(sp^3) centres in coupling reactions.[2] The conformational stability of boronic esters, however, has resulted in primarily stereospecific transformations of enriched boronic esters,[3] and there are few examples of enantioselective methods.

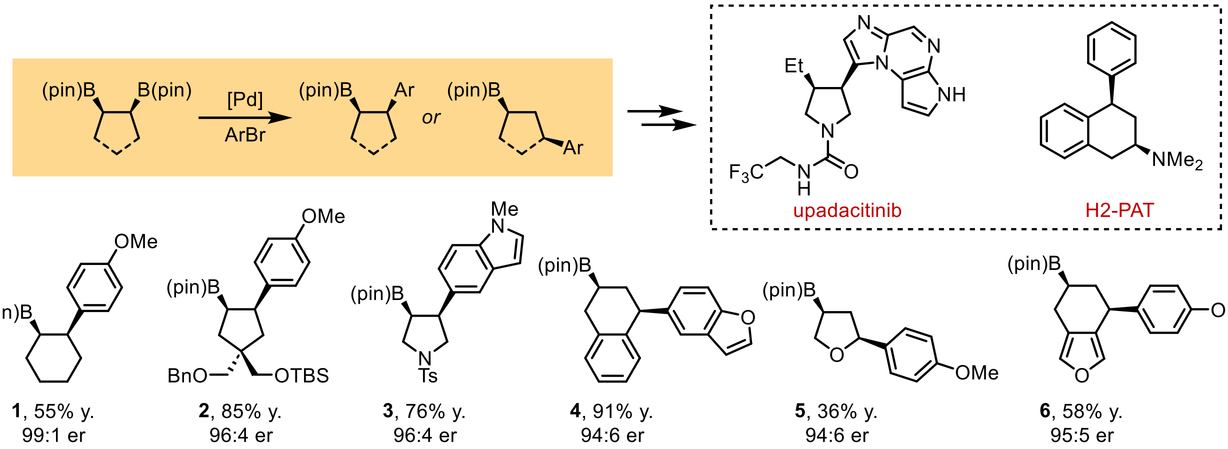

Figure 1: Enantioselective Suzuki-Miyaura cross coupling reaction and potential applications.

Previous work found vicinal bis(boronic) esters undergo rapid relative to the mono(boronic ester),[4] and we envisioned this be leveraged for the desymmetrisation of all-secondary *meso* bis(boronic esters). The developed reaction conditions are amenable for coupling an array of aryl and heterocyclic electrophiles with diverse functional groups to (hetero)cyclic *meso* bis(boronic) esters. Notably, substrate electronics and steric encumbrance could be leveraged to promote coupling immediately after transmetalation (Figure 1,**1−3**),[5] or after chain-walking to a predictable, distal location (Figure 1, **4−6**). This provides access to two functional group patterns as the remaining enriched boronic ester can be readily transformed, providing in-roads to complex structures from easy-to-access substrates.

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P082

Next-generation DNAzymes

T.Behn[1], S. Kath-Schorr*[1]

Universität zu Köln, Institut für Organische Chemie

e-mail: t.behn@uni-koeln.de

The significance of nucleic acid therapeutics has been on the rise in the past years, most notably due to the mRNA vaccines and antisense technology.

DNAzymes are catalytically active DNA molecules that were developed in the 1990s through *in vitro* selection and evolution.[1] Although many DNAzymes that have since been developed exhibit promising properties *in vitro* to be used as therapeutics, none have been utilized as such, yet. This is primarily the low *in vivo* activity, as well as the low biostability observed in cell experiments[2]. Among the most promising candidates are the 8-17 and 10-23 DNAzyme, which are able to cleave RNA in a site-specific manner, utilizing metal cofactors such as magnesium ions.[1]

Given that the development of DNAzymes utilizing only natural building blocks has reached its optimum, incorporation of artificial modifications to enhance the DNAzymes properties is of great interest. However, rational design approaches were limited for a long time due to the unknown structure and mechanism of action, which was only recently elucidated for the 10-23 DNAzyme by *Etzkorn* et al.[2,3]

Furthermore, the authors introduced a base modification to the catalytic active site that increased catalytic activity by six-fold.[2] This presents a first rational design approach to improve the properties of the 10-23 DNAzyme, which is further explored in this project. For this purpose, organic synthesis is utilized to create novel building blocks for solid-phase DNA synthesis using phosphoramidite chemistry. In combination with well-established modifications used in other nucleic acid therapeutics, next-generation DNAzyme variants are developed to enabling therapeutic applications of this promising technology.

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P083

THIOPHENE-BODIPY BASED COF MATERIALS

B. Çoşut [1], B. Topaloğlu Aksoy [1], Buse Köse [2], E. Tanrıverdi Eçik [2]

[1] Gebze Technical University, Department of Chemistry, Kocaeli, 41400 TURKEY
[2] Atatürk University, Department of Chemistry, Erzurum, 25240 TURKEY

Covalent organic frameworks (COFs), regarded as innovative smart materials in the new generation, have garnered significant interest ever since Yaghi et al. first reported them in 2005.[1] They belong to a category of crystalline porous organic polymers characterized by permanent porosity and meticulously ordered structures. Specifically, the tunable pore size and structure of COFs, coupled with their enduring porosity, extensive surface area, thermal stability, and low density, enhance the functionality and broaden the range of applications for these materials.[2]

Boron complexes of dipyrromethene compounds are termed 'bordipyrromethene' or simply BODIPY compounds. They are extensively utilized owing to their high molar absorption properties, elevated fluorescence quantum yields, and prolonged lifetime of singlet excited states.[3] Through the synthesis of tetrastyryl BODIPY derivatives, which exhibit absorbance and emission in the near-infrared wavelengths due to their extensive conjugated structure, a novel covalent organic framework (COF) structure was created using an anhydride coupling element.

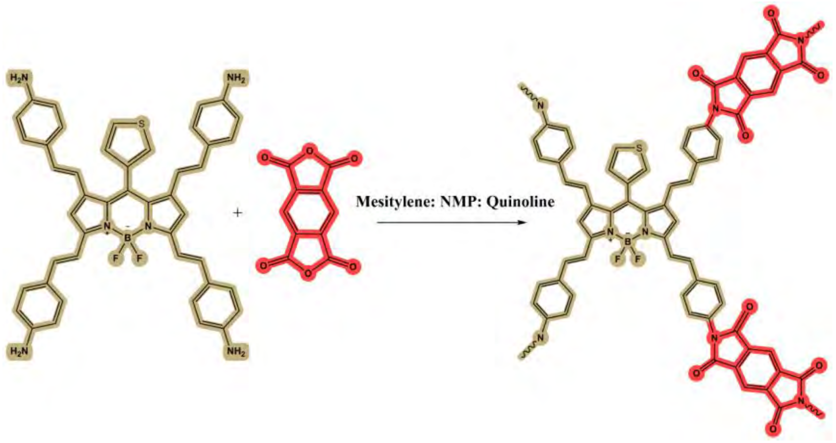

Figure 1: Synthesis outline of the Thiophene-BODIPY based COF material

The primary objective of this study is to fabricate porous covalent organic structures, wherein the pore size and conjugation can be manipulated through the utilization of BODIPY-based photosensitizers known for their highly effective photonic applications.

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P084

A metabolomics approach to uncover new natural products from human-derived streptomycetes

Nicola U. Thome[1,2], Joleen Masschelein[2], Gilles P. van Wezel[1]

[1] Department of Molecular Biotechnology, Institute of Biology, Leiden University, The Netherlands

[2] Laboratory for Biomolecular Discovery & Engineering, VIB-KU Leuven Center for Microbiology, KU Leuven, Belgium

The growing incidence of diseases caused by multidrug-resistant pathogens is a major threat to human health and necessitates the discovery of novel antibiotics. Many of the antibiotics we use in the clinic are natural products produced by Actinobacteria. Nevertheless, even the genomes of well-known antibiotic producers harbor numerous not yet characterized biosynthetic gene clusters (BGCs), which correspond to so far undiscovered natural products. In the search for novel natural products with potential antibiotic activity, omics techniques such as metabolomics play an important role. A major challenge though is to dereplicate known natural products in metabolomics data as spectral databases are incomplete. Here, we're using molecular networks built from untargeted LC-MS/MS data,[1] to explore the chemical space of a collection of Actinobacteria. We currently focus on an outstanding collection of streptomycetes isolated from the human lung.[2]

As many BGCs are silent under routine laboratory growth conditions, we also grow the bacteria in different conditions, and then screen for changes in the metabolomes, similar to the high-throughput elicitor screening (HiTES) approach.[3] In particular, we want to provide insights into how those human-derived strains respond to a range of human-associated molecules and hormones. With this approach, we aim to identify compounds that activate the biosynthetic potential of Actinobacteria and apply them to find new antibiotics. The findings may furthermore indicate mechanisms that also play a role in microbiome-host interactions and they may facilitate the development of drug-producing probiotics.

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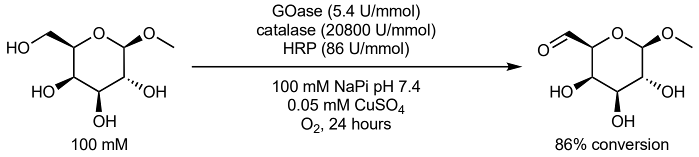
P085

Galactose Oxidase Catalyzed Stereocontrolled Petasis Reaction

Yawen Zhang [1] and Scott E Schaus [1]

[1] *Boston University, Chemistry Department, Boston, USA*

The Petasis reaction is a multicomponent reaction using amine, aldehyde, and aryl-boronic acid to form substituted amines.[1] The enantioselectivity of the Petasis reaction have been controlled mainly in two ways: chiral catalyst and chiral starting material. However, efficiently synthesize chiral aldehydes at high enantiopurity remained challenging. Our research is advancing towards using enzymatic catalysis to acquire α-hydroxy aldehydes used in the stereocontrolled Petasis reaction. Enzymatic catalysis has the potential to easily achieve high enantioselectivity in an economically advantageous and environmentally friendly way.
To establish the one-pot stereoselective Petasis reaction, we must investigate the structure and catalytic reaction of Galactose Oxidase (GOase). The reaction conditions of GOase-catalyzed C-1 modified D-galactopyranose derivatives were established and optimized. Under the established benchmark reaction condition, methyl-β-D-galactopyranoside displayed 86% conversion into corresponding aldehyde after 24 hours of reaction at room temperature (Scheme 1). Substrate table of C-1 modified D-galactopyranose derivatives were developed to explore the significance of the side chain at C-1 position. The product of each D-galactopyranose derivatives was characterized as the aldehydes with no carboxylic acid side product. We found that the C-1 position of D-galactopyranose affected the enzyme-substrate interaction but did not inhibit the oxidation reaction. The same D-galactopyranose derivatives were also tested on electrochemistry setup followed by the same workup procedure. The electrochemical reaction setup achieved comparable conversion and similar substrate specificity but did not show absolute advantage over the benchtop reaction setup.



Scheme 1: GOase oxidation of methyl-β-D-galactopyranoside under benchmark condition.

Besides sugar alcohol substrates, we attempted to oxidize 1,2-diols into α-hydroxy aldehydes, the reactants in the stereocontrolled Petasis reaction. Literatures have revealed the kinetic resolution of single alcohol substrates while no literature has reported GOase oxidation of 1,2-diols. So far, no 1,2-diols substrates tested were oxidized by GOase on benchtop or electrochemical setup. Additionally, we found that 1,2-diols were oxidized into racemic carboxylic acids directly by the platinum electrodes. This finding contradicted with the result reported in the literature, which claimed that electrodes do not cause overoxidation of primary alcohols. Future studies focusing on developing mutated GOase may allow high enantiopurity in the kinetic resolution of diols. Once we develop an effective way of obtaining the α-hydroxy aldehydes, we will proceed to perform the GOase catalyzed stereoselective Petasis reaction.

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P086

Anti-Markovnikov Functionalisation of Olefins

Alexandra Matei,[1] Sebastian B. Beil[1], Ben L. Feringa[1]

[1] *University of Groningen, Stratingh Institute for Chemistry, Groningen, The Netherlands*

Classical oxidations of terminal olefins generally follow Markovnikov selectivity, producing ketones, known as the Wacker oxidation or process.[1]-[3] However, anti-Markovnikov oxidations of terminal alkenes are interesting for organic chemists, as they give direct access to aldehydes, which are versatile building blocks in numerous organic synthetic applications. While several Pd-catalyzed methodologies for the regioselective oxidation of alkenes have been developed, the number of more sustainable direct oxidative protocols is limited.[3]-[8] A combination of metal-redox catalysis and photochemistry to achieve anti-Markovnikov oxidations of alkenes into aldehydes would present a highly desirable and sustainable alternative towards synthesizing this important class of chemical intermediates. This project focuses on the development of new methodologies taking advantage of highly active catalysts to avoid the stoichiometric use of oxidants in order to achieve direct anti-Markovnikov oxidation of ideally unactivated terminal alkenes.

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P087

Obtaining new silicon phthalocyanines as sensitizers with high singlet oxygen efficiency using the combined effect of light and ultrasound

Kevser Celep [1], Göknur Yaşa Atmaca[1], Ali Erdoğmuş [1]

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

Cancer, a complex and widespread disease, has challenged the medical field with its diverse manifestations and treatment resistance [1,2]. Photodynamic therapy (PDT), sonodynamic therapy (SDT), and the new innovative, combined sono-photodynamic therapy (SPDT) have emerged as promising approaches in this endeavor, harnessing the power of reactive oxygen species (ROS) and, more specifically, singlet oxygen to induce cytotoxic effects on malignant tumor cells [3,4].

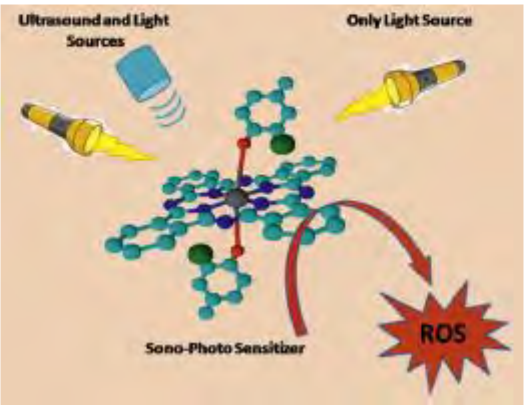

Figure 1: Depiction of PDT and SPDT on silicon phthalocyanine sensitizer

In this context, this study aimed to synthesize, characterize, and evaluate the photochemical, sonochemical and sono-photochemical properties of novel silicon phthalocyanines carrying halogen substituents (2-Chloro-4-methylphenol and 2-Bromo-4-methylphenol silicon phthalocyanines). In this study the highest singlet oxygen generation was observed in sono-photochemical studies ($\Phi_{\Delta SPDT}$=0.80, 0.82 respectively**)**. This is because with the combination therapy of light and sound better therapeutic results are achieved. The synthesized compounds demonstrate notable promise as potential candidates for sono-photosensitizers, suggesting the possibility of increased cytotoxicity and enhanced therapeutic effectiveness in cancer treatment.

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P088

Development, synthesis, and characterization of antifouling hydrogels for wound dressings

Aliia Ibragimova [1], Ulrich Jonas [1]

[1]*University of Siegen, Department of Chemistry and Biology, Siegen, Germany*

Healing of chronic wounds or ulcers is significantly slower and complex compared to acute wounds since they do not follow a regular wound recovery course.[1] The treatment of chronic wounds is challenging and requires the development of specialized wound dressings.[2,3] Ideally, an adequate dressing needs to protect the wound from contamination mechanically, and also prevent infection by the supply of antimicrobials or antibiotics without provoking antimicrobial resistance.[2,4] It should provide a moist environment preventing wound desiccation, whilst stimulating healing by a steady and effective release of the applied bioactive substances.[4] In other words, an adequate dressing should not only protect the wound but also actively promote the natural healing process.[2,4] Hydrogels are very promising materials for wound dressing applications, since they provide a moist environment, can be loaded with bioactive components, and maintain substantial drug release. Some are oxygen and nutrients permeable, non-toxic, biocompatible, biodegradable, and do not trigger an immune response of the organism.[2,4] In this work, acrylamide- and 2-oxazoline-based hydrophilic monomers and photocrosslinking comonomers were synthesised and copolymerized via free radical (FRP) and microwave-assisted cationic ring opening polymerisation (CROP) respectively. The polymers were structurally characterized and used for fabrication of hydrogel-based composite membranes. The ability of a protein-based drug to diffuse through the membrane and its interaction with the hydrogel material was assessed with UV-VIS spectroscopy and circular dichroism by the use of a diffusion cell and in solution with free polymers in a pharmaceutical buffer. Thus, current results show that the hydrogel-based composite membrane is generally suitable for protein-based drugs since the polymeric materials did not demonstrate an apparent interaction with polypeptide-compounds.

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P089

Uncovering the mechanism of photodenitrogenation reactions with NAMD simulations

Leticia A. Gomes[1], Steven A. Lopez[1]

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

Photochemical reactions are examples of green chemistry used to synthesize strained molecules under mild conditions.[1,2] One example is the light-promoted denitrogenation of bicyclic azoalkanes, which can produce bicyclo[2.1.0]pentane with retained or inverted diastereoselectivity.[3,4] However, the mechanism behind these reactions has been disputed for over six decades. To solve the longstanding mechanistic questions, we employed multireference calculations and non-adiabatic molecular dynamics (NAMD) simulations on a series of diazabicyclo[2.2.1]heptenes. Our simulations provide detailed information on their photophysical properties, reactivities, and mechanistic pathways. We used complete active space self-consistent field (CASSCF) calculations with an (8,9) active space and ANO-S-VDZP basis set. CASSCF energies were corrected with XMS-CASPT2(8,9)/ANO-S-VDZP. For the parent and two derivatives with methyl substituents the lowest excitations are $n_{NN}(\sigma_{CN}) \rightarrow \pi^*$ and range from 3.94 – 3.97 eV. We created 500 initial conditions using Wigner sampling for each molecule and implemented the fewest switches surface hopping NAMD simulations. We identify four pathways post S_1/S_0 intersections: the reversal to reactant, the inversion product exo-housane, the retention product endo-housane, and a diradical intermediate. Our analysis indicated that the diazoalkanes undergo asynchronous conical intersections, where one σ_{CN} bond breaks along the S_1 and the other σ_{CN} breaks after hopping to the S_0 (Figure 1).

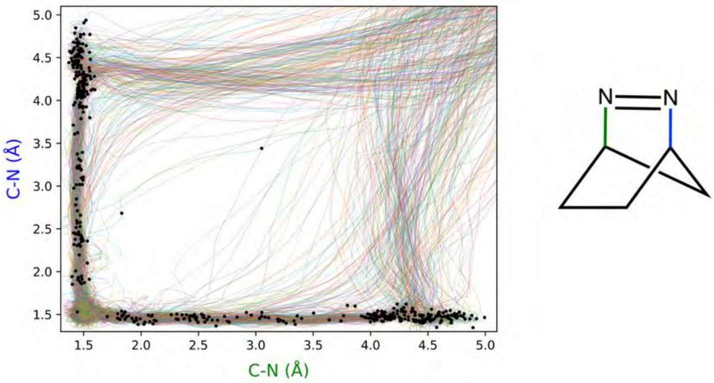

Figure 1 - σ_{CN} bonds plotted against each other for diazabicyclo[2.2.1]heptene. The bond lengths we calculated are depicted. The solid multicolor lines on each plot show the bond lengths over time, and the dots represent the S_1/S_0 surface hopping points for each trajectory.

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P090

Controlling the Dispersity of Antimicrobial Copolymers

Jan Kurki[1], Anne Lehnen [1], Matthias Hartlieb [1]

[1] University Potsdam, Institute of Chemistry, Potsdam, Germany

Millions of lives are saved annually, by the routine use of broad-spectrum antibiotics. Due to the misuse of medicines by people in many different areas, more and more multiresistant bacteria are spreading. AMR (antimicrobial resistance) was directly responsible for 1.27 million global deaths in 2019 and contributed to 4.95 million deaths. The WHO expects AMR and the consequences of AMR to cost the lives of 10 million people a year by 2050 [1].

Antimicrobial peptides (AMP) and especially the resulting antimicrobial polymers (AP) are a variant to combat this problem. Many different studies have shown that the architecture of AP has an influence on their effectiveness against bacteria and their toxicity against mammalian cells. An example of this would be Anne and coworkers who showed the advantage of graft polymers over linear chains [2] and Boyer et al. showing the influence of topology and chain length on bacteria [3].

I want to show here that I can use the XPI raft, a variant of the RAFT polymerisation that avoids many of its limitations [4], to easily produce polymers (linear chains and bottlebrushes) where I can specifically adjust the dispersity and then test their biological properties and compare them with each other (Figure 1).

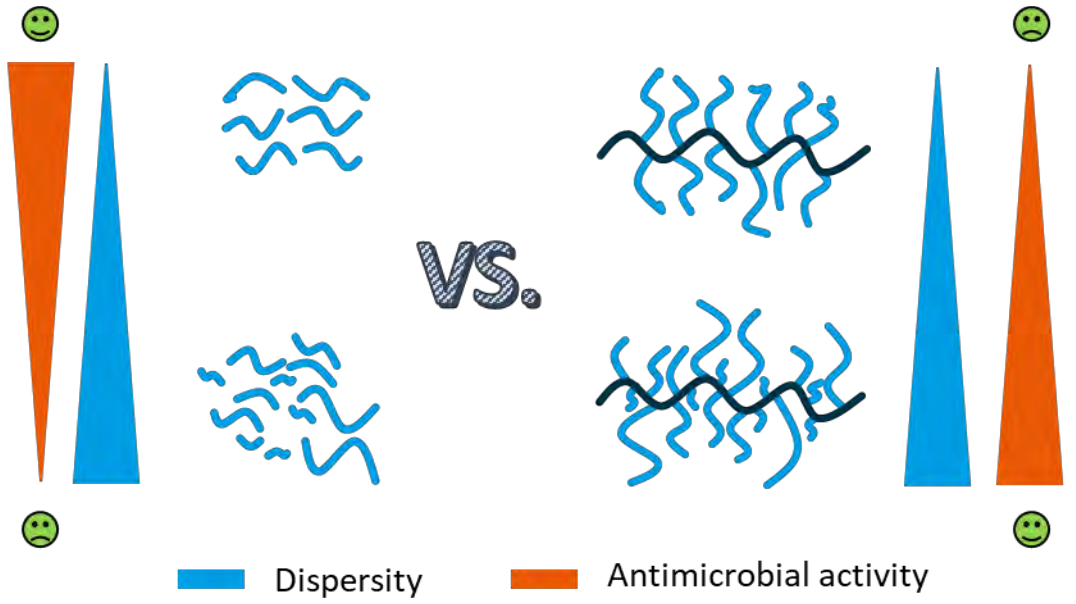

Figure 1: Difference of Dispersity for linear Chains and Bottlebrushes and the change in properties.

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P091

Autophagic, Mitocondrial and Apoptotic Effects of Drug-Loaded Nanoparticles on Lung Cancer Cells

Fatma Şayan POYRAZ [1], Banu MANSUROĞLU [2]

[1] *Yildiz Technical University, Faculty of Art&Science, Department of Molecular Biology and Genetics, Istanbul, Turkey.*

Polymeric carrier systems are frequently used in cancer treatment recently to develop an alternative strategy to commonly used traditional treatments such as radiotherapy and chemotherapy, which have very high side effects. One of the most preferred polymers when creating polymeric carrier systems is PLGA (poly-lactide-co-glycolide) polymer, which is biocompatible, biodegradable, and easily eliminated from the body.[1] Gentisic Acid (GA), an aspirin metabolite, is a phenolic compound with a very broad pharmacological spectrum containing two -OH groups in para positions. It is particularly powerful in terms of antioxidant and free radical scavenging activities and has been proven to show pro-apoptotic and antiproliferative effects in various cancerous tissues.[2] 5-Fluorouracil is a kind of antimetabolite that was synthesized as a rationally designed anticancer agent, functions as a pyrimidine antagonist, and is widely used in the treatment of various types of cancer. The mechanism of action of 5-FU consists of interfering with DNA synthesis and mRNA translation.[3] Conventional treatments of cancer, especially chemotherapy, negatively affect not only cancer cells but also healthy cells of the body. Our technique aims to encapsulate the 5-fluorouracil molecule, a chemotherapeutic agent with strong and highly toxic properties in cancer treatment, and the Gentisic Acid molecule, a phenolic acid derivative, into PLGA. Through a controlled release mechanism, 5-fluorouracil and gentisic acid substances damage cancerous cells without damaging healthy cells. In this context, nanoparticles were synthesized by the Double Emulsion Solvent Evaporation Method, and as a result of the analysis, the size was found 192.27 nm, the zeta potential was -24.3 mV and PDI values were 0.110. The nanoparticles' homogeneous, spherical structure and average size were also confirmed by Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM) analyses. The cytotoxic effect of nanoparticles was determined by the MTT method in A549 human lung cancer cells and healthy fibroblast cells in comparison with free substances. In the analyses performed on A549 cells using the IC50 values obtained for free substances and nanoparticulate form, the effects on apoptotic effect by DAPI staining, on autophagic vesicles by Acridine Orange staining, and on mitochondrial membrane potential by JC-1 staining were examined. When compared to free drug forms, it was determined that the nanoparticulate system was more effective in apoptosis, autophagy and mitochondrial membrane activity and killed cancer cells.

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P092

Water soluble cyclotriphosphazene derivative including indole group

Ceylan Mutlu Balcı [1], Duygu Palabıyık [1], Serap Beşli [1]

[1] *Gebze Technical University, Faculty of Basic Science, Kocaeli, TURKEY*

Cyclotriphosphazene can easily perform substitution reactions with organic molecules, including many functional groups because of its electronic structure and the atoms' position on the ring. This allows for the synthesis and creation of new hybrid molecules with desired properties. [1] Long-chain glycol derivatives are very important in anticancer drug studies and biological active molecules synthesis due to their water-soluble properties. In this study, firstly, a glycol derivative, which facilitates water solubility, was substituted on one side of the phosphazene ring, and an indole derivative, which has a high potential for anti-tumour activity, was substituted on the other side.

First of all, the triple cis non-geminal product was isolated from the possible product mixtures to be obtained by interacting cyclotriphosphazene, trimer with triethylene glycol monomethyl ether. [2] The triple cis non-geminal compound is interacted with ethoxy methyl indole, a heterocyclic aromatic derivative, in the presence of NaH at a 1:3 mol ratio, synthesized a new cyclotriphosphazene derivative (Figure 1).

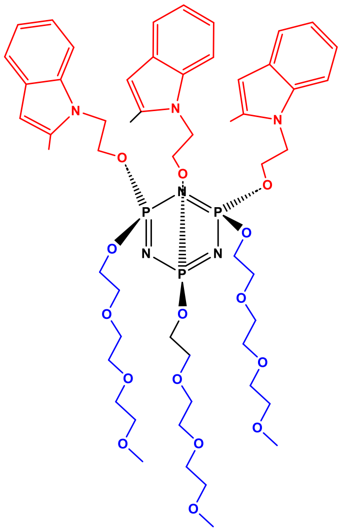

Figure 1: Water soluble cyclotriphosphazene derivative

The characterization of the newly synthesized compound was performed by MALDI-TOF, ^{31}P and ^{1}H, ^{13}C NMR spectroscopy, and the structure of suitable single-crystal ethoxy methyl indole was determined by single-crystal X-Ray crystallography. Anti-tumour activity study of syntheses molecule will be conducted by in vitro methods using colorectal cell lines.

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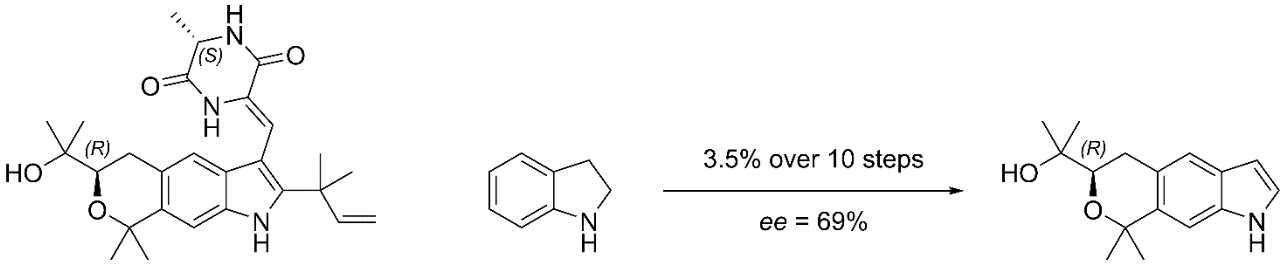
P093

Synthesis of the pyrano[4,3-*f*]indole section of variecolorin K from the halotolerant fungus *Aspergillus variecolor*

Alexandra Dierks[1], Marvin Fresia[1], Thomas Lindel[1]

[1] TU Braunschweig, Institute of Organic Chemistry, 38106 Braunschweig, Germany

The isoechinulin-type alkaloids variecolorin A−L (K: **1**) from the fungus *Aspergillus variecolor* display radical scavenging, UV-A-protecting, immunosuppressive, and antibacterial activity. The variecolorins share a prenyl-derived side chain at C5, that may be oxygenated and chlorinated in different ways. As in the structurally related echinulins, a *tert*-prenyl group is installed at C2 and the tryptophan head forms an alkylidene diketopiperazine unit with alanine.[1]



1 **2** **3**

Figure 1: Variecolorin K (**1**), and enantioselective synthesis of an advanced intermediate **3** starting from indoline (**2**).

The main goal of this synthesis was to determine if the sterically crowded dihydropyran ring could be assembled. The first target was the synthesis of 6-iodo-5-prenylindoline by aza-Claisen rearrangement from a *tert*-prenylated amine. The more direct strategy involved a reductive iodonio-Claisen rearrangement, which would follow an S_N2' attack of allyl silane or prenyl silane at an λ^3-iodane was found to be inferior. Next, the dihydropyran ring was assembled. Sharpless AD of the prenyl group, followed by protection of the resulting diol as an acetonide, and subsequent hydroxyisopropylation of C6 through iodine/lithium exchange afforded the required cyclization precursor. Deprotection of the acetonide under acidic conditions led to cyclization. The pyrano[4,3-*f*]indole section **3** of variecolorin K was obtained from indoline (**2**) for the first time in 10 steps and 3.5% overall yield (*ee* = 69%).
Elimination of *p*-toluenesulfinic acid, followed by Danishefsky *tert*-prenylation at C2, formylation at C3, and condensation with the in situ-formed diketopiperazine formed from L-alanine and glycine, could give variecolorin K (**1**).[2] An alternative strategy involves a Horner-Wadsworth-Emmons reaction with the formyl group at C3 and a diketopiperazine derived from commercially available *N*-carboxybenzyl-*α*-phosphonoglycine trimethyl ester and L -alanine.[3]

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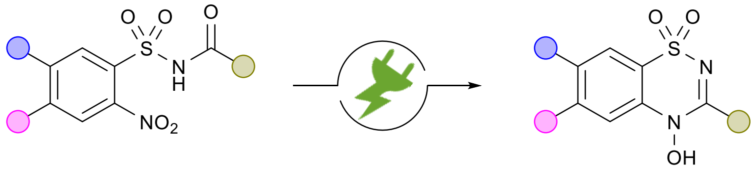
P094

Cathodic Nitro Reductions a Versatile Tool in Heterocycles Synthesis Exemplified by 4*H*-4-Hydroxybenzo[*e*]-1,2,4-thiadiazine-1,1-dioxides

Tobias Prenzel [1], J. Winter [1], Tom Wirtanen [1], María de Jesús Gálvez-Vázquez [1], Kamil Hofman [1], Dieter Schollmeyer [1], Siegfried R. Waldvogel [1,2,3]

[1] Johannes Gutenberg-University Mainz, Department of Chemistry, Mainz, Germany
[2] Max-Planck-Institute for Chemical Energy Conversion, Muelheim an der Ruhr, Germany
[3] Karlsruhe Institute of Technology, Institute of Biological and Chemical Systems – Functional Molecular Systems (IBCS-FMS), Karlsruhe, Germany

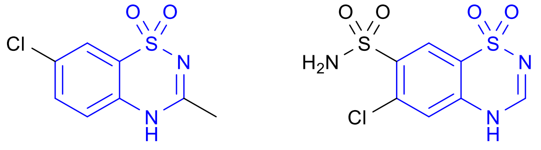
Nitrogen containing heterocycles represent an important structural motif in natural products and blockbuster pharmaceuticals. Therefore, their synthesis plays a crucial role in the chemical industry.[1] The *N*-hydroxy motif is often found as major metabolite for such nitrogen containing heterocycles. As an innovative tool, electrochemistry enables direct access to *N*-hydroxy heterocycles via direct reduction of easily accessible nitro arenes. By utilizing electrical current from renewable resources as an inherently safe and inexpensive reagent, electrochemistry contributes to an increased sustainability of chemical processes.[2,3]



Key Facts

- 44 diverse examples up to 97% yield
- common electrolyte system
- carbon-based electrodes (metal-free)
- scalable and easy to conduct
- simple constant current electrolysis
- easy work-up protocol

Benzo[e]-1,2,4-thiadiazine-1,1-dioxide based APIs



Diazoxide™ *Diuril*™

Figure 1: Highly selective, scalable electrosynthesis of 4*H*-4-hydroxybenzo[e]-1,2,4-thiadiazine-1,1-dioxides.

As an example, 4*H*-4-hydroxybenzo[*e*]-1,2,4-thiadiazine-1,1-dioxides are based on a widely found structure motif for pharmaceutical applications having an additional unique exocyclic N-O bond which are not accessible by conventional synthetic routes. A highly selective electrosynthesis of 4*H*-4-hydroxybenzo[*e*]-1,2,4-thiadiazine-1,1-dioxides by direct reduction in almost quantitative yields is presented. The electro-synthetic protocol was applied to more than 40 diverse examples highlighting the versatility of this method. Furthermore, the technical relevance was demonstrated by two multi-gram scale syntheses.[4]

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P095

A PEPICO study of key reaction steps in toluene combustion

Ewald Keksel [1], Sebastian Kluge [1], Domenik Schleier [1], Martin Höner [1], Yasin Karakaya [1]
Thomas Bierkandt [2], Markus Köhler [2], Tina Kasper [1]

[1] *Technical Thermodynamics, Paderborn, University, Paderborn, Germany*
[2] *Institute of Combustion Technology, German Aerospace Center (DLR), Stuttgart, Germany*

Full surrogates consist of a limited variety of hydrocarbons and are crafted to replicate the combustion characteristics found in actual fuels. Toluene commonly serves as a significant element in these surrogate fuels. Consequently, the primary oxidative routes of toluene have undergone extensive investigation, yielding numerous kinetic modeling documented in literature[1-3]. Within fuel surrogates, the oxidation chemistry of toluene interacts with those of other hydrocarbons present in the mixture. In toluene flames containing added butadiene or acetylene in this study, an acceleration of toluene decomposition due to the low-temperature reactions initiated by the additive in both scenarios is observed. Significant intermediates involved in the decomposition of toluene in low-pressure laminar flames are identified through comparison of flame-sampled mass-resolved threshold photoelectron spectra obtained via photoion coincidence spectroscopy at the Swiss Light Source (Figure 1) to literature photoionization data.

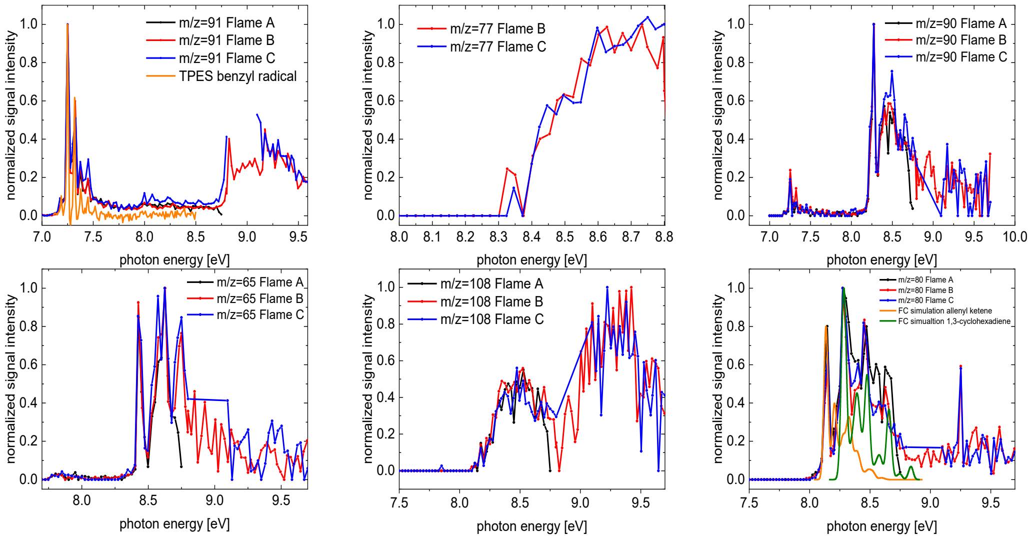

Figure 1: ms-TPES of m/z=91 of the benzylradical, m/z=77 of the phenylradical, m/z=90 of the fulvenallene, m/z=65 of the cyclopentadienylradical, m/z=108 of the 2-methylphenol and m/z=80 of the cyclohexadiene.

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P096

Valorization of Poly(Lactic Acid)/Polyaniline Composite in the Removal of Hazardous Indigo Carmine Textile Dye from Wastewater

Birol Isik[1], Volkan Ugraskan[1]

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

Due to the limited availability of accessible water sources on the earth's surface, which is largely covered with water, and considering the importance of water resources today, conservation has become a highly significant issue. Recently, approximately 10% of the over 600,000 tons of dye produced annually, from a production capacity standpoint, is directly discharged as waste into water sources.[1,2] With industrial advancements, the toxicity, stability, and persistence of wastewater discharged directly into water sources are causing irreversible problems for human and environmental health. While various methods are used for wastewater treatment, the adsorption method is widely employed due to its advantages such as low cost and easy application. In the adsorption method, various materials are used as adsorbents. Recently, the preparation of adsorbents that are low-cost, biodegradable, and sustainable has come to the forefront.[3,4]

In this study, a conductive polymer, polyaniline, was synthesized. Then, composites were prepared by adding varying amounts of polylactic acid, a biodegradable polymer, into the gel at different mass ratios. The performance of the prepared composites in removing indigo carmine textile dye from aqueous solutions was evaluated. In the initial stage of the study, optimum conditions such as the amount of adsorbent, contact time, temperature, and initial concentration, were determined using the prepared adsorbents. Afterward, adsorption studies were conducted, and the raw data were applied to Langmuir, Freundlich, Dubinin-Radushkevich, and Temkin isotherm models, as well as *pseudo-first-order* and *pseudo-second-order* kinetic models. It was determined that the Langmuir isotherm model was suitable for the adsorption of indigo carmine dye onto the prepared composites, and the process followed the *pseudo-second-order* kinetic model. Additionally, the adsorption process was conducted at different temperatures to examine the adsorption thermodynamics. From the thermodynamic results, it was found that the adsorption process is exothermic and spontaneous.

This research has been supported by Yildiz Technical University Scientific Research Projects Coordination Department. Project Number: FKD-2023-5843.

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P097

Synthesis and ultrafast spectroscopy of a novel derivative of the carotenoid astaxanthin

Emrah Özcan[1], Radek Litvín[1], Tomas Polivka[1]

[1]*Faculty of Science, University of South Bohemia, Branišovská 31, České Budějovice, Czechia*

Carotenoids, the most abundant pigments in nature, serve various functions, including photoprotection, light harvesting, and antioxidant activity. The latter plays a crucial role as a protective mechanism against several human diseases, such as cancer, atherosclerosis, and macular degeneration [1]. Astaxanthin, a carotenoid, features two oxygen atoms on each cyclohexene ring in the form of a keto and hydroxyl group, enabling chemical modification by attaching various functional groups to the terminal rings (Figure 1). Specifically, keto groups can undergo imine reactions with primary amines [2, 3]. The cyclohexene ring structure is identical to that of many hydroxyl quinones and α-hydroxy-ketones, known for their high biological activity. The modification of astaxanthin is expected to alter its photophysical properties [3]. In this study, we have examined a new derivative of astaxanthin using ^{1}H NMR, FT-IR, Mass, and HPLC spectroscopy. Photophysical properties of the astaxanthin derivative were investigated through UV-VIS absorption and ultrafast time-resolved transient absorption spectroscopy techniques. The data show that astaxanthin can be successfully modified with organic compounds, resulting in significant changes in absorption spectra. These changes in spectroscopic properties were corroborated by transient absorption data, revealing that the astaxanthin derivative's S1 lifetime, approximately 5 ps for astaxanthin, was shortened to 1.3 ps, indicating a profound effect of modification on the excited state dynamics.

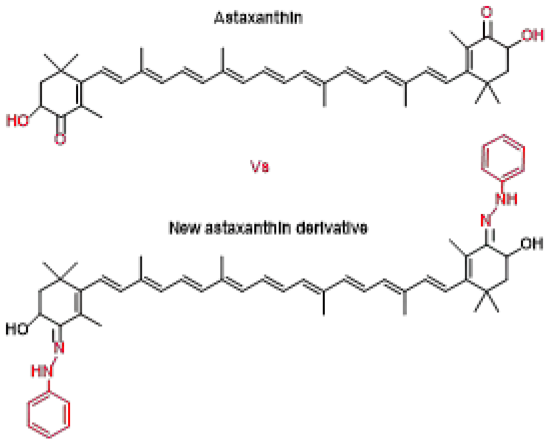

Figure 1: Astaxanthin and new astaxanthin derivative are shown.

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P098

Application of Surface Plasmon Resonance in Marine Chemistry

Arne Estelmann[1], Willem Marz[2], Ralf Prien[1]

[1] Leibniz-Institute for Baltic Sea Research, Rostock, Germany
[2] University of Rostock, WG Water Management, Rostock, Germany

The majority of chemical analytics of seawater is still based on the measurement of discrete samples in the laboratory. However, traditional sampling is time-consuming, expensive and cannot resolve small-scale processes or transient events. Thus, there is an urgent need for the development of in situ sensors, which require the implementation of new technologies.[1]

Surface Plasmon Resonance (SPR) has become a powerful analytical method in pharmaceutics and biochemistry. SPR sensors are widely used for highly sensitive, fast, specific and label-free quantification. Although most SPR setups are designed for laboratory use, increasingly smaller and more portable prototypes have been presented in the last decades.[2,3]

However, despite its potential for in situ use, SPR based sensing is not established in marine sensor technology, yet. To date, we know of only two in situ applications of SPR in marine chemistry, of which only one prototype was submersible in the sea.[4,5]

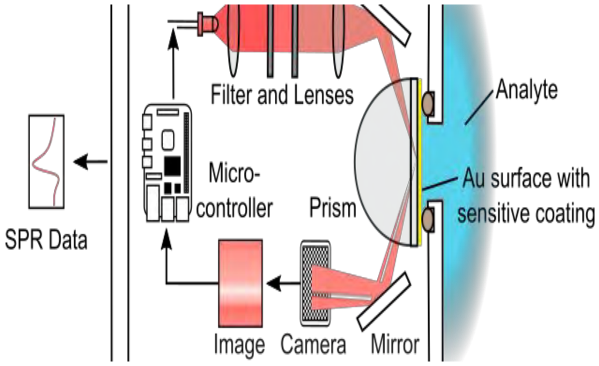

Fig. 1: Example of a submersible SPR prototype.

On our poster, we will look at the advantages and disadvantages of this technique based on literature examples and our own experience.[6,7] We will discuss potential analytes and parameters, for which in situ SPR sensors offer an advantage over currently available sensors. Finally, we will present our approach to a submersible chemical sensor and the status of our current work.

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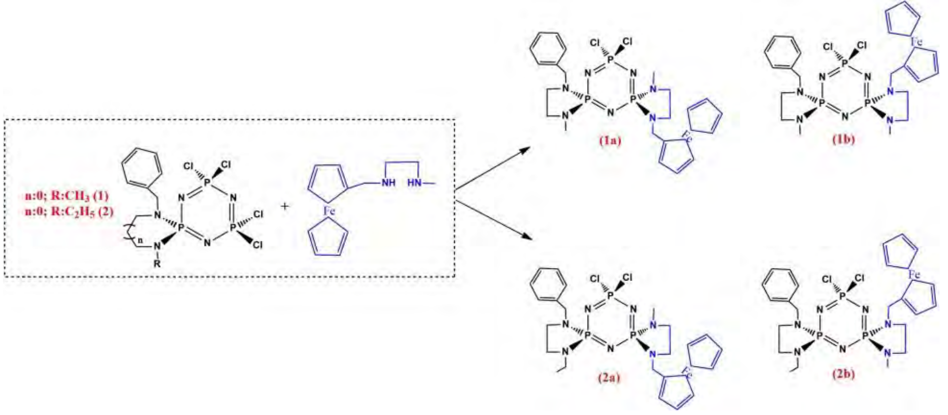
P099

Unsymmetrically-substituted dispirocyclotriphosphazenes with ferrocenyl pendant arms: synthesis, characterization, antituberculosis activities and phototunable charge storage studies

Reşit Cemaloğlu [1], İpek Berberoğlu [1], Mehtap Yakut [1], Arzu Binici [1], Nuran Asmafiliz [1], Zeynel Kılıç [1], Remziye Güzel [2], Gülbahar Erdal [3], Hülya Şimşek [4] Tuncer Hökelek [5]

[1] *Ankara University, Department of Chemistry, Ankara, Türkiye*
[2] *Dicle University, Department of Chemistry, Diyarbakır, Türkiye*
[2] *Dicle University, Dept. of Molecular Biology and Genetics, Diyarbakır, Türkiye*
[4] *Bozok University, Department of Medical Microbiology, Yozgat, Türkiye*
[5] *Hacettepe University, Department of Physics, Ankara, Türkiye*

Hexachlorocyclotriphosphazene, $N_3P_3Cl_6$, (**HCCP**) have been used as a platform to produce many organic and inorganic substituted trimeric phosphazene derivatives.[1,2] Unsymmetrical dispirophosphazenes having one ferrocenyl-armed spiro group have not been encountered in the literature. Ferrocenyldiamines are known to exhibit antituberculosisactivity against *M. tuberculosis* H37Rv. Therefore, it is thought that new drug-active molecules can be obtained by appending trimeric phosphazene with ferrocenyldiamines. To achieve this aim, primarily, trans (**1a** and **2a**) and cis (**1b** and **2b**) unsymmetrical dichlorodispiro(N/N)cyclotriphosphazenes were obtained from ferrocenyl-diamines and benzyl-pendant armed tetrachloromonospirophosphazenes (**1** and **2**) (Scheme).[3] Spectroscopic characterizations of these compounds were performed. All unsymmetrically substituted phosphazenes are expected to be racemic mixtures due to two different stereogenic P-centers. In addition, the molecular and crystal structure of cis-**1b** was elucidated via single-crystal X-ray crystallography. The antituberculosis activities of **1a** and **1b** against *M. tuberculosis* H37Rv (ATCC 27294) strain were also investigated. In addition,the compounds (**1a** and **1b**) were characterized by voltammetric methods to understand theelectrochemical behavior of the ferrocene-modified dispirophosphazenes. To determine thephototunable charge storage properties of the dispirophosphazenes (**1a** and **1b**), their memory functions were investigated.



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P100

Increasing the Singlet Oxygen Formation of BODIPY Derivative by Sonophotochemical Technique

Ceren Can Karanlık [1,2], rkan Karanlık [1,2], Ali Erdoğmuş [1,2]

[1] *Yildiz Technical University, Department of Chemistry, Istanbul, Turkey*
[2] *Health Biotechnology Joint Research and Application Center of Excellence, Istanbul, Turkey*

The therapeutic approach for cancer utilizing Photodynamic Therapy (PDT) and Sonodynamic Therapy (SDT) depends on three essential elements: the stimulation method (light or ultrasound), a sensitizer, and singlet oxygen ($^1O_2$). The effectiveness of the treatment relies on the synergistic interaction of these factors, as no single component alone is adequate for successful treatment. While each component plays a crucial role with distinct tasks, singlet oxygen, categorized as a reactive oxygen species (ROS), emerges as particularly pivotal in the overall treatment process. In both methods, singlet oxygen plays a critical role. Higher singlet oxygen quantum yield is indicative of increased therapeutic efficacy. Consequently, researchers in this field primarily focus on enhancing the singlet oxygen quantum yield of sensitizers, aiming to maximize their therapeutic potential [1-3].

PDT and SDT share substantial similarities, differing primarily in the nature of the stimulating agent employed for the sensitizer. PDT utilizes a specific wavelength of light, whereas SDT relies on low-frequency ultrasound to activate sensitizers. Sonophotodynamic Therapy (SPDT), a novel combination method, has been devised to address and overcome the drawbacks associated with both individual methods in practical application [4,5].

In this study, we present the synthesis, characterization and photophysicochemical/sonophotochemical studies of BODIPY derivative. Our results show that BODIPY derivative can be a potential sensitizer in PDT and SPDT applications based on singlet oxygen quantum yield.

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P101

A Ratiometric Nanosensor Approach for DNA Detection via Single Stranded DNA-Labelled Carbon Quantum Dots

Dilek Öztürk [1], Mahmut Durmuş [1]

[1] *Gebze Technical University, Faculty of Science, Kocaeli, 41400 Türkiye*

DNA-based biosensors have gained significant attention due to their high sensitivity, selectivity, and ability to detect various target analytes[1]. Carbon-based quantum dots are zero-dimensional nanomaterials with excellent properties such as low cost, simple synthesis, low cytotoxicity, good biocompatibility, high photo and chemical stability, tunable excitation and emission spectra, and surface modification processes[2,3]. This study presents a ratiometric nanosensor approach for detection of DNA using carbon quantum dots (CQDs). Carbon quantum dots were synthesized using citric acid and ethylenediamine by a microwave method. At the end of the reaction, a brown crystal (similar to an amber crystal) was obtained, which was dissolved in water and purified with a dialysis membrane. The surface of the synthesized carbon quantum dots was conjugated with single-stranded DNA (ssDNA). Ethidium bromide is a specific dye that increases fluorescence by binding to double-stranded DNA[4]. The fluorescence intensity of the blue-emissive CQDs-ssDNA nanoprobe system was quenched with ethidium bromide. Then, when complementary ssDNA was added to the system, red emissive ethidium bromide interacted with hybridized double-stranded DNA by strong intercalating. Thus, a ratiometric nanosensor system was developed by increasing the red emission fluorescence intensity of ethidium bromide while the blue emission of CQDs decreased.

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P102

Photoswitches for dynamic supramolecular modulation of proteins

Alisa-Maite Kauth[1], Antonio Bietti[2], Katrin Hommel[2], Shirley Knauer[2], Thomas Schrader[2], Bart Jan Ravoo[1]

[1] University of Münster, Center of Soft Nanoscience, Münster, Germany
[2] University of Duisburg-Essen, Essen, Germany

Over the past decades, the incorporation of azo-compounds as photoswitches in biological systems has generated increasing attention due to the desire of creating photocontrollable biotargets. Besides the recent promising developments in this field, there are still problems with the reversibility, photoisomerization and half-life times of the developed azobenzenes.[1] Arylazopyrazoles (AAPs) show improved photophysical properties, especially a reversible quantitative photoisomerization in both directions (E-to-Z with UV light, Z-to-E with green light), slow thermal relaxation and good stability in water. AAPs have proven themselves in a broad variety of applications, such as host-guest complexes, hydrogels and surfactants, enabling phototunable properties.[2]

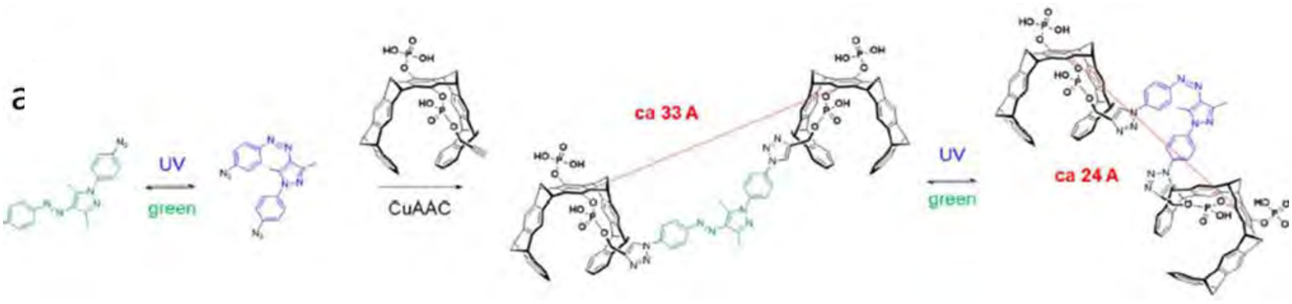

Figure 1: Photoswitchable divalent tweezer.

For example, AAPs can be used as active compounds in photocontrollable supramolecular ligands for proteins. We synthesized different “clickable” AAPs, which can be easily conjugated to various ligands using copper alkyne azide click reaction (CuAAC). Our photoswitches were combined with molecular tweezers to create phototunable protein binders that interact selectively with lysines exposed on the protein surface. These photoswitchable tweezer molecules show a good stability over several switching cycle, beside a long half-life time of the Z state. The distance between the molecular tweezer was tuned by using AAPs with different length. These tweezer-AAPs were used for manipulating protein binding since the isomers inhibit protein functions differently.

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P103

Adsorptive Removal of Methylene Blue Dye from Aqueous Solutions Using SnS_2-Filled Sodium Alginate Composites

Volkan Ugraskan[1], Birol Isik[1]

[1] *Yildiz Technical University, Faculty of Arts & Science, Department of Chemistry, Istanbul, Turkey*

Water pollution has recently emerged as an important global problem due to the increased need for clean water resources as a result of rapid industrialization and urbanization.[1,2] Contaminated water sources also seriously threaten human health. Organic dyes are typically toxic and resistant to degradation due to their structure and physicochemical properties, and therefore, dyes that are highly carcinogenic and mutagenic organic pollutants pose a significant health hazard to living things in the biosphere.[3] The adsorption method is considered the most widely used and promising method for the removal of dye-containing wastewater due to its high efficiency, low cost, ease of use and reliability, simplicity of regeneration, sludge-free operation, and the absence of harmful and hazardous end products.[4]

In this study, the performance of SnS_2-filled sodium alginate (SA/SnS_2) composites in removing methylene blue (MB) dye from aqueous solutions by the adsorption method was examined. Firstly, studies were carried out on different parameters such as temperature, pH, contact time, amount of adsorbent, and dye concentration to determine the optimum conditions for the adsorption process. The adsorption data were applied to various adsorption isotherms and kinetic models. In addition, the nature of the adsorption process was determined by calculating the thermodynamic parameters with the data obtained. The results showed that SA/SnS_2 composites effectively adsorbed MB dye.

This research has been supported by Yildiz Technical University Scientific Research Projects Coordination Department. Project Number: FKD-2023-5840.

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P104

Synthesis and function of a non-ribosomal peptide produced by entomopathogenic bacteria

Trinetri S. M. Goel [1], Yonggyun Kim [2], Helge B. Bode [1,3,4]

[1] *Max Planck Institute for Terrestrial Microbiology, 35043 Marburg, Germany. * E-Mail: trinetri.goel@mpi-marburg.mpg.de*
[2] *Andong National University, College of Life Sciences, Department of Plant Medicals, Andong 36729, Korea*
[3] *Goethe-University Frankfurt, Molecular Biotechnology, Department of Biosciences, 60438 Frankfurt am Main, Germany*
[4] *Philipps-University Marburg, Chemical Biology, Department of Chemistry, 35043 Marburg, Germany*

Natural Products, such as non-ribosomal peptides are small chemical compounds produced by living organisms to serve higher functions such as signaling and defense.[1,2] These organisms obtain an evolutionary advantage due to the high chemical diversity of natural products inducing unique bioactive functions.[1,3] Nevertheless, the bioactivity and function of many natural products remain unknown until today.[4] Non-ribosomal peptides are a class of natural products that are biosynthesized by large multi-enzyme complexes called non-ribosomal peptide synthetase.[1] GameXPeptides are a class of highly abundant non-ribosomal peptides from entomopathogenic *Xenorhabdus* and *Photorhabdus* bacteria.[5] To investigate their bioactivity, biological function, and molecular targets, these cyclic peptides and their functionalized derivatives have been chemically synthesized and tested in biological and biochemical assays. The bioactivity test results indicate that GameXPeptides have insecticidal properties by suppressing the immune system.

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P105

Ultrathin surface-attached hydrogel coatings for intentional implant removal

Laura Finck [1], Valentin Hagemann [2], Sebastian Polarz [2], Henning Menzel [1]

[1] Technical University of Braunschweig, Institute of Technical Chemistry, Braunschweig, Germany

[2] Leibniz University Hannover, Institute for Inorganic Chemistry, Hannover, Germany

The further development of implant materials is of highest interest to make implants safer. Not only the prevention of infections, but also the easy removal of implants should be considered. For an intentional implant removal, a reversible nanoparticle glue shall be developed. It is known in the literature that nanoparticles can glue synthetic hydrogels with other hydrogels or soft tissue,[1] and this gluing can be reversed by high temperatures. The use of superparamagnetic core-shell nanoparticles should make it possible to release the adhesion with an alternating magnetic field (AMF) as an external trigger. The superparamagnetic nanoparticles can generate heat through magnetic hyperthermia[2] so that the bonded materials can be separated. This process thus supports explantation (see figure 1).

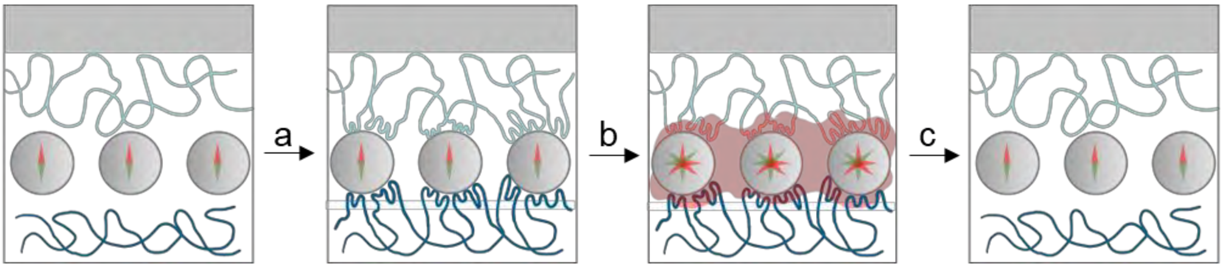

Figure 1: Schematic diagram for a facilitated removal. a: Adsorption of the polymer chains on the surface of magnetic nanoparticles, b: AMF as trigger for magnetic heating, c: polymer adsorption gets less.

An ultrathin hydrogel shall be covalently bonded to the implant surface for the coating. For this purpose, a copolymer was prepared that can bind to the implant surface (titanium) via a phosphonate group. Furthermore, a photo-crosslinkable group like arylazide and hydrophilic groups to form a hydrogel were incorporated. The coatings were characterized via in-situ ellipsometry measurements. Layer thicknesses of between 40 and 140 nm in the dry state can be adjusted via the concentration of the spin-coating solution. The coatings swell in water to about twice their thickness depending on the crosslinking density. The immobilization of different nanoparticles can be confirmed by SEM.

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P106a

The Young Chemists Network Frankfurt

Annabelle Brauel [1], Nils Wegerich [1], Leon Kirschner [1]

[1] *Goethe University, Young Chemists Network, Frankfurt, Germany*

The Frankfurt Regional Network of the Young Chemists Network (JCF) currently has 26 active members (Fig. 1A) who organize and host various events throughout the year. In addition to regular networking meetings, the summer colloquium, and the Christmas lecture (Fig. 1C), this also includes the Frankfurt job fair for scientists (Fig. 1B and 1D), which attracts over 2,000 visitors every year, a stand at the Night of Science and a volleyball tournament in cooperation with the Student Representative Body for chemistry. Last year, in 2023, the JCF Frankfurt also organized a workshop in cooperation with the journal *Angewandte Chemie* and further exciting events are already being planned for the coming year.

Figure 1: A) Group photo with active members. B) Information stand at the Frankfurt job fair for scientists. C) Christmas Lecture. D) Group photo from the Frankfurt job fair for scientists.

P106b

24. Frankfurter Jobbörse für Naturwissenschaftler:innen

Leon Kirschner, Annabelle Brauel, Badria Ali, Nils Wegerich

JCF Regionalforum Frankfurt am Main

Save the date for the 6th and 7th November 2024! The 24th *Frankfurter Jobbörse für Naturwissenschaftler:innen* is taking place again. The program starts with plenty of workshops and seminars on Wednesday, November 6. There will also be the opportunity to have your application documents and CVs checked by trained career consultants. You can find out more about the various events at https://jobboerse-ffm.de/. Registration is expected to begin in early October.

On Thursday, November 7, the fair day will follow, with around 20 companies and associations taking part. From 9:30 a.m. to 4:30 p.m., a wide variety of companies from the chemical industry, pharmaceuticals, and life sciences, as well as start-up companies, business consultancies and patent law firms will be presenting themselves.

In addition to the classic exhibition stands, many companies will also give a short presentation about their company. There will also be the opportunity to have professional application photos taken. Finally, our program will end with a public job interview, which you can attend live.

P107

Spectroscopic and Crystallographic Properties of New Ferrocenylcyclotriphosphazene with Functional Amine Terminated

Nagihan BAYIK TÜLÜCE [1], Nuran ASMAFİLİZ [2], Gön l YENİLMEZ ÇİFTÇİ [1]

[1] Gebze Technical University, Department of Chemistry, Kocaeli, Türkiye
[2] Ankara University, Department of Chemistry, Ankara, Türkiye

Hexachlorocyclotriphosphazene (trimer, $N_3P_3Cl_6$) is a rigid inorganic heterocyclic structure with six chlorine members, consisting of P-N centers.[1] It can be easily functionalized by nucleophilic substitution reactions of the chlorine atoms in its structure. Thus, cyclotriphosphazene has the feature of functionalization with different substituents and gaining different properties depending on the types of substituents.[2,3] Ferrocene-based compounds have attracted widespread attention in various flame retardant polymeric materials. The presence of many active functional groups ($-NH_2$) in cyclotriphosphazene provides the opportunity for chemical reaction modifications and the preparation of polymeric materials.[4]

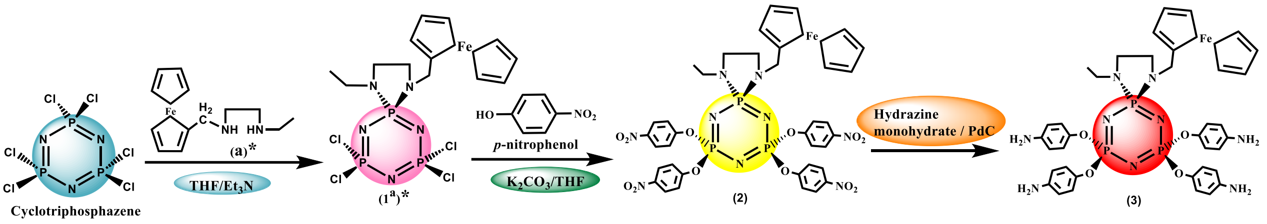

Figure 1: Reaction Pathway of Functional Amine-Terminated Ferrocenylcyclotriphosphazene.

In this study, a new functional amine-terminated ferrocenylcyclotriphosphazene was synthesized for polymer reactions planned to be used in the field of innovative materials. For this, firstly, mono(ferrocenyldiamino)spirocyclotriphosphazene (**1a***) was synthesized from the reaction of ferrocenyldiamine (**a***) with trimer. Then, from the nucleophilic substitution reaction of **1a*** with p-nitrophenol give the tetra(p-nitrophenoxy)mono(ferrocenyldiamino)spirocyc-lotriphosphazene (**2**). In the last stage, the hydrolysis of **2** in the presence of hydrazine monohydrate and PdC was carried out and the compound **3** with functional amine terminated was successfully obtained. The structures of the new synthesized phosphazenes (**2** and **3**) were characterized using mass, NMR (^{1}H, ^{31}P) and IR spectroscopy techniques. Also, the crystal structures of the new compounds were elucidated by X-ray crystallography technique.

This study is supported by Gebze Technical University Scientific Research Projects Coordination (Project Number: 2023-A-102-02). Nagihan Bayık is supported by the Turkish Higher Education Council's 100/2000 PhD fellowship program.

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P108

The green chemistry approach behind the DeNO$_x$-DePM project

Andreas Fuchs [1], Marc O. Schmid [1], Ulrich Vogt [1]

[1] *University of Stuttgart, Institute of Combustion and Powerplant Technology, Stuttgart, Germany*

Green chemistry describes the environmentally friendly chemical synthesis in order to minimize the environmental pollution. This can be achieved by substitution towards non-toxic starting materials, especially if they come from renewable sources, reduction in pollution by side products and products, as well as optimizing the energy use in the synthesis.[1,2]

The DeNO$_x$-DePM project aims at a combined reduction in the emissions of particulate matter and NO$_x$, which are pollutants that are emitted during the combustion of biomass, which represents in the heating sector the most important renewable energy source with 84 %.[3] This shall be achieved by an innovative procedure for the flue gas cleaning in which a catalytic active additive is added directly into the flue gas in order to be removed together with the particulate matter at a mesh filter in order to develop a catalytic active filter cake. The filter including the filter cake removes particulate matter as well as NO$_x$ simultaneously. After reaching a critical thickness resp. a critical pressure drop is reached at the filter, the filter can be cleaned by a jet-pulse in reverse direction while the powerplant can be kept running.[4] The catalytic additive will be a supported transition metal oxide low temperature SCR catalyst, which is more environmentally friendly than the industrial used V_2O_5-based catalyst.[5] This shall not only be achieved by the chemicals used for the synthesis, but also by the use of microwave technology.

By substituting chemicals in order to improve the environmental friendliness of the SCR catalyst while also lowering the temperature in which the reaction will take place as well as the use of microwave technology in the synthesis, this project is taking a green chemistry approach.

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P109

Singlet Oxygen Generation by Monostyryl NI-BODIPY-Fullerene Triads for Degradation of ABDA

Ezel Öztürk Gündüz[1], Ümmügülsüm Büyükpolat[1], Hande Eserci Gürbüz[1], Elif Okutan [1]

[1] *Gebze Technical University, Department of Chemistry, Kocaeli, Turkey*

Fullerene-C_{60} is the smallest stable and most abundant member among the fullerene family. Electron deficient fullerene-C_{60} tend to give addition reactions with nucleophiles hence C_{60} can functionalize with various substituents which leads to prepare fullerene-based systems for various applications.[1] Preparation of dyads, triads or polyads is a design approach that unify more than one or two molecules in a single platform. This strategy has been implemented to develop chromophore-based molecules for light harvesting systems. Borondipyrromethene (BODIPY) dyes have been studied extensively due to their unique photophysical properties.[2]

In this study, new naphthalimide-BODIPY-C_{60} triad, bearing NI unit on the styryl position of BODIPY core was prepared and subjected to photophysical, and photochemical studies. Structural characterization of the triad was investigated via mass, ^1H and ^{13}C NMR spectroscopy techniques. The photophysical properties were investigated by the methods of steady-state UV–Vis absorption and fluorescence spectroscopy. The new triad exhibited strong absorption bands with quenched fluorescence character, and good singlet oxygen generation ability as expected from a good photocatalyst.

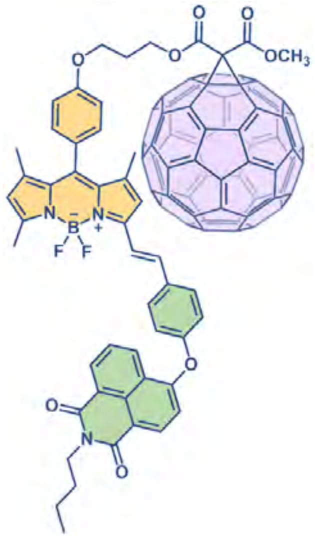

Figure 1: Molecular structure of NI-BODIPY-C_{60} triad.

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P110

How can we formulate green biosurfactants?

Janine Birnbach [1,2], Peter Schmiedel [2], Matthias Karg [1]

[1] Institut für Physikalische Chemie I, Heinrich-Heine-Universität Düsseldorf, Germany
[2] LRS-Physical Chemistry, Henkel AG & Co. KGaA, Düsseldorf, Germany

Surfactants are used in many applications in our everyday life. However, they are often still made from fossil resources, which contradicts a circular economy. Biosurfactants may be a solution because they are made from renewable resources, sometimes even waste streams, in a fermentation process. Moreover, they have a low toxicity and easy biodegradability. Despite this, the replacement of fossil-based surfactants by biosurfactants has not been very successful in the past years since biosurfactants have different, often more complex, structures and compositions leading to different physico-chemical properties. Therefore, simple substitution is not possible and the physico-chemical properties of biosurfactants need to be evaluated and understood, especially in multi-component systems, which are common in formulations.

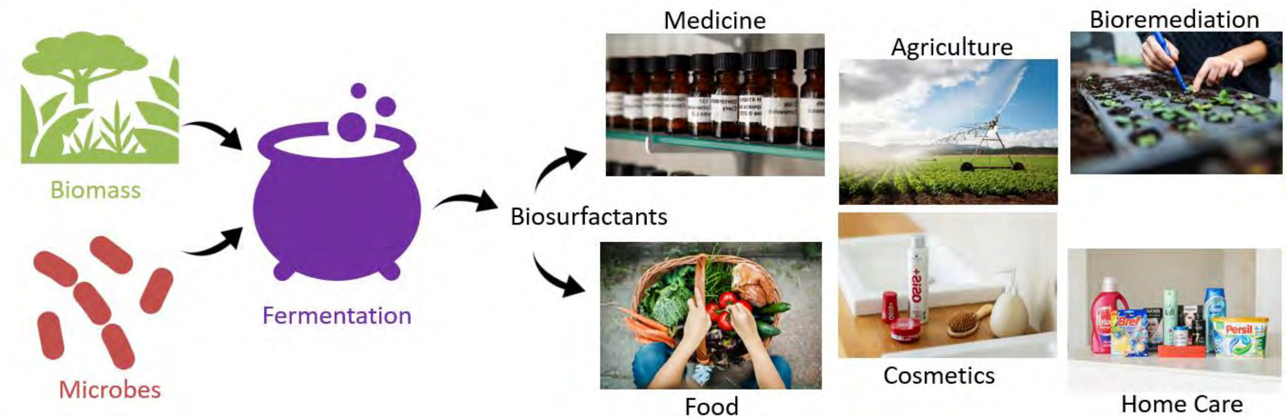

Figure 1: origin of biosurfactants and examples of their applications

This is why we focused on the state-of-the-art in the multi-component phase behavior of biosurfactants with a comprehensive literature review including our own works. We found that biosurfactants form a wide variety of different structures, some of which are not observed for conventional surfactants. Furthermore, the emulsion properties vary depending on the type of biosurfactant, the type of oil and whether or not a secondary surfactant is used. It can be concluded that individual formulations with biosurfactants need to be developed for different applications [1].

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P111

Conformational Analysis of Cb- and TIB-terminated Diketides during Spartein-Free, Highly Stereoselective 1,2-Metallate Rearrangements

Yannick Linne[1], Maike Birkner[1], Jan Flormann[2], Daniel Lücke[1], Jörg August Becker[2] and Markus Kalesse[1]

[1] Leibniz University, Institute for Organic Chemistry, Hanover, Germany
[2] Leibniz University, Institute for Physical Chemistry and Electrochemistry, Hanover, Germany

Stereotriards containing allylic alcohols as well as methods to generate such structures are of high interest for the synthesis of natural products. The Hoppe−Matteson−Aggarwal rearrangement, a 1,2 metallate rearrangement, typically performed with + or – sparteine to ensure the formation of the desired diastereomer, can be used to synthesise such structures. However, during the natural synthesis of Condochloren A by Linne et al., it was discovered that in the absence of spartein both higher yields and diastereselectivites could be achieved for the reaction of a vinylic boron ester and Cb- or TIB-terminated diketides.[1] Additionally, the dicetide termination decides if the Felkin to the Anti-Felkin product primarily is formed. The aim of this work thus is to systematically analyse in which reaction steps the stereoselectivity is introduced, using experimental and theoretical methods. [2]

10-c1 [CYLview of **10-c1**] [Newman projection of **10-c1**]

Figure 1: Lowest energy rotamer of Cb-terminated diketide 10 with Felkin and anti-Felkin sphere. [2]

To analyse the directing effects during the Lithiation of the protected large diketides, a hybrid conformational sampling based on metadynamics was performed on DFTB and DFT levels of theory. Boltzmann factors were used to select significantly populated rotamers of two Cb- and two TIB-terminated diastereomers (at the reaction temperature of -78°C) as shown in Figure 1 for one dicetide. These structures were then used to rationalise the observed diastereomer selectivities during spartein-free lithiation and subsequent borylation. For Cb-terminated diketides, the selectivity of the lithiation is found in the final product as well, indicating a retention process. For TIB-terminated diketides, both retention and inversion processes are likely to occur during borylation.

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P112

Functionalization of detonation nanodiamond with small zwitterionic peptides to control interactions and improve biocompatibility in biological environments

Elisabeth Mayerhoefer[1], Harsh Nitin Dongre[2], Daniela Elena Costea[2], Anke Krueger[1,*]

[1] Institute of Organic Chemistry, University of Stuttgart, Stuttgart, Germany
[2] The Gade Laboratory for Pathology and Center for Cancer Biomarkers (CCBIO), Department of Clinical Medicine, University of Bergen, Bergen, Norway

Nanodiamond (ND) particles offer a versatile platform for numerous applications in biomedical research owing to their unique surface chemistry and low toxicity profile. These utilizations demand a precise interplay of the ND surface with the cellular target, which can be achieved by decorating the surface with tailored functionalities.[1] When exposed to physiological environments, however, the uncontrolled adsorption of proteins or lipids on the particles' surface and the resulting high agglomeration tendency is a major obstacle. This process of protein corona formation not only reduces the accessibility of attached functional elements for cellular interactions but can also lead to alterations of the uptake mechanism into cells.

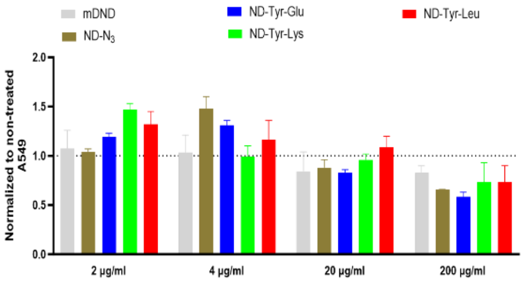

Figure 1: Cytotoxicity assay (results obtained by manual cell counting) of precursor particles and all dipeptide functionalized NDs on A549 cells.

We recently reported on the successful implementation of a complex zwitterionic functionalization to address these undesired effects and enhance colloidal stability.[2] To provide a more efficient and low-cost zwitterionic functionalization with sufficient biocompatibility, we now covalently conjugated detonation nanodiamond (DND) with three different zwitterionic dipeptides. Here, we report the synthesis of these dipeptide functionalized NDs and investigations on their behavior in solutions of varying pH values and in serum protein-containing cell culture media. When incubated with normal and malignant human cells in 2D and 3D cell cultures, the NDs exhibit significantly different biocompatibility and cellular uptake depending on the attached dipeptide (Figure 1). With these findings in hand, we could identify particular dipeptides facilitating not only stable, protein corona-free ND particles, but also low toxicity and sufficient uptake. This opens the way to more complex functionalization patterns using a multimodal approach combining protein repelling properties with additional functionalities for e.g., targeting or drug delivery.

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P113

Azobenzenes with Fluorinated Alkyl Chains to Explore Non-Covalent Interactions

Silke Müsse[1,2], Hermann A. Wegner[1,2]

[1] Institute of Organic Chemistry, Justus Liebig University Giessen
Heinrich-Buff-Ring 17, 35392 Gießen (Germany)
[2] Center of Materials Research (ZfM/LaMa), Justus Liebig University
Heinrich-Buff-Ring 16, 35391 Giessen (Germany)

Contrary to common belief, recent research shows that fluorine-fluorine interactions in perfluorocarbons can exhibit a significant dispersive potential, only limited by geometric constraints.[1] This study utilised azobenzene (AB) as a molecular wind-up meter (MWM)[2,3], to explore fluorine-fluorine (**Fehler! Verweisquelle konnte nicht gefunden werden.**).

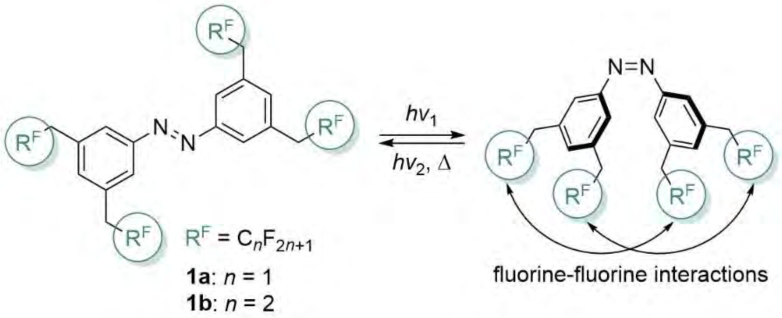

Figure 1: AB 1 as an MWM to study fluorine-fluorine interactions.

The synthesis of AB **1a**, involving late-stage functionalisation *via* Suzuki-Miyaura coupling, proves valuable for introducing methylene-bridged trifluoromethyl groups to AB. Kinetic investigations of CF_3-AB **1a** in comparison to its hydrocarbon analogue in both *n*-octane and perfluorooctane showed that CF_3-AB **1a** exhibit shorter half-lives possibly due to steric repulsion from the larger CF_3 group. Both compounds showed enhanced half-lives in their opposite solvent, indicating that the (*Z*)-state is more stabilised due to decreased destabilising solvent-solute interactions. This investigation provides fundamental insights into fluorine-fluorine interactions, which reach into all areas, such as drug design, catalysis, or material science.

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P114

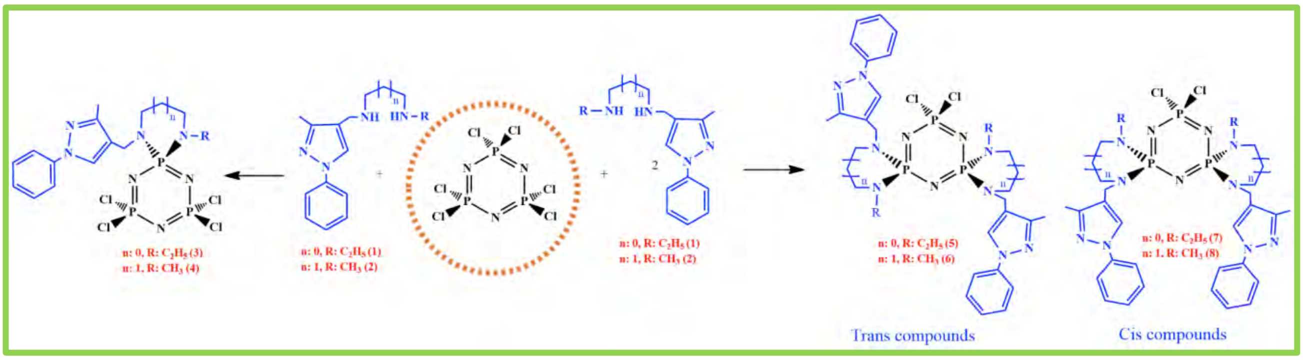
Synthesis and investigation of structural and biological properties of mono and dispiro(pyrazolinediamino)cyclotriphosphazenes

Nuran Asmafiliz [1], Reşit Cemaloğlu [1], Zeynel Kılıç [1], Leyla Açık [2], Tuncer Hökelek [3]

[1] Ankara University, Department of Chemistry, Ankara, Türkiye
[2]Gazi University, Department of Biology, Ankara, Türkiye
[3]Hacettepe University, Department of Physics, Ankara, Türkiye

Cyclotriphosphazenes have gained an important place in biological activity studies.[1,2] Heterocyclic compounds are also involved in the development of pharmacologically active derivatives. One of these compounds is the 5-membered pyrazole molecule. Pyrazole and its derivatives have been used as pharmacophores in the structure of natural and synthetic compounds with anti-inflammatory, anticancer, antibiotic, antibacterial, antifungal and analgesic activities.[3,4]

In this study, mono and dispiro(pyrazolinediamino)phosphazenes were obtained to determine their spectroscopic, stereogenic and biological properties. Firstly, the reactions of 3-methyl-1-phenyl-pyrazole-4-carboxaldehyde with the aliphatic diamines produced the pyrazolinediamines (**1** and **2**). Then, the mono (**3** and **4**) and dispiro (pyrazolinediamino)phosphazenes (**5**-**8**) The structures of **3**-**8** were elucidated by various spectroscopic methods. However, the dispirophosphazenes are expected to have stereogenic phosphorus atoms and the chiral properties of these compounds were investigated by CSA-added ^{31}P NMR spectra. On the other hand, the antimicrobial activities of cyclophosphazenes and their interactions with pBR322 plasmid DNA were examined.



The authors acknowledge the Scientific and Technical Research Council of Turkey Grant No. 123Z057.

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P115

Adsorption of Hazardous Methylene Blue Dye Using *Vitis vinifera* L. from Wastewater

Fatih Cakar[1], Ayse Erdogan Cakar[1], Birol Isik[1], Ozlem Cankurtaran[1]

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

The grapevine leaves, known by their Latin name *Vitis vinifera* L., are a plant that grows by wrapping around surrounding plants, with woody branches and deciduous leaves in winter. Although primarily native to southwest Asia, it grows almost everywhere in the world. The leaves of *Vitis vinifera* L. are rich in tannins, flavonoids, and proanthocyanidins, and also contain abundant organic acids, lipids, enzymes, and vitamins. Since ancient times, the leaves of *Vitis vinifera* L. have been used in medicine for various reasons such as their biological activities including hepatoprotective and spasmolytic effects, as well as hypoglycemic and vasodilatory effects, and their antibacterial, antifungal, anti-inflammatory, antinociceptive, antiviral, and especially antioxidant properties.[1,2]

In this study, the leaves of *Vitis vinifera* L., which are low-cost, abundantly grown almost everywhere in the world, readily available, and have a fibrous structure, were evaluated within the scope of zero waste. These leaves were used as adsorbents for the removal of methylene blue dye from wastewater. To conduct the adsorption studies effectively and effectively, optimum conditions such as initial pH, contact time, initial concentration, and adsorbent dose were determined. After determining the optimum conditions, adsorption experiments were performed, and the raw data obtained were applied to isotherm and kinetic models.[3,4] To evaluate the efficiency of adsorption, the experimental results were applied to Langmuir, Freundlich, and Dubinin-Radushkevich (D-R) isotherm models. From the results, it was determined that the adsorption of methylene blue onto *Vitis vinifera* L. leaves fit the Langmuir isotherm model. For evaluating the adsorption kinetics and mechanism, experimental data were applied to *pseudo-first-order* and *pseudo-second-order* kinetic models, revealing that the adsorption process followed the *pseudo-second-order* kinetic model. The characterization of the prepared adsorbents was conducted using FTIR-ATR analysis before and after adsorption.

This research has been supported by Yildiz Technical University Scientific Research Projects Coordination Department. Project Number: FBA-2023-5826.

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P116

Pillar[5]quinone synthesis and investigation of its usability potential in aqueous zinc batteries.

Yasemin SOLMAZ[1], Nazmiye KILIÇ[1], Burcu ÜNAL[2,3], Özlem SEL[4,5], Rezan DEMİR-CAKAN[2,3], Serkan YEŞİLOT[1]

[1] Department of Chemistry, Gebze Technical University, Kocaeli, Turkey
[2] Department of Chemical Engineering, Gebze Technical University, Kocaeli, Turkey
[3]Institute of Nanotechnology, Gebze Technical University, Gebze, Kocaeli, Turkey
[4]Chimie du Solide et de l'Energie UMR 8260, Collège de France, 75231 Paris Cedex 05, France
[5]Réseau sur le Stockage Electrochimique de l'Energie (RS2E) CNRS FR 3459, 80039 Amiens Cedex, France

Energy crisis and environmental pollution resulting from energy consumption have become serious problems today. Zinc-ion rechargeable batteries, one of the new and most promising alternative energy storage technologies, have recently attracted great attention because zinc is abundant in natural resources, is safe, and is cost-effective compared to expensive lithium-ion batteries[1]. There is increasing interest in organic cathode materials used as an alternative to inorganic cathode materials in battery applications[2]. Pillar[n]quinone attracts great attention because the multiple carbonyl groups in its structure can serve as more than one active centre during battery applications and the molecular weight per active centre is as low as possible.

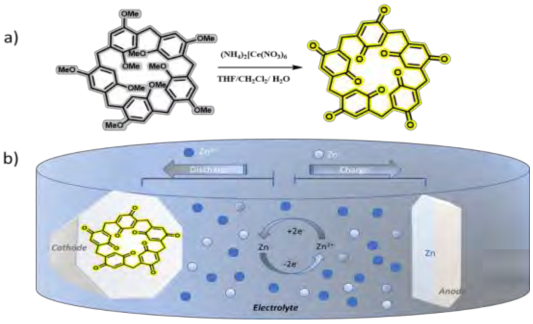

Figure 1. a) Pillar[5]quinone synthesis, b) Application as cathode in zinc ion batteries.

In the study, pillar[5]quinone compound was synthesized in accordance with the literature and characterized using appropriate characterization methods (Figure 1a)[3]. The obtained pillar[5]quinone compound was used as a cathode material in aqueous zinc ion batteries and its electrochemical performances were examined(Figure 1b). Electrochemical mechanism of pillar[5]quinone was investigated using the Density Functional Theory methode. We wish to thank TÜBİTAK 1001 (222-Z-042) project and TUBITAK ULAKBIM, High Performance and Grid Computing Center (TR-Grid e-Infrastructure) for the calculations.

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P117

Synthesis, Characterization and Evaluation of Photophysicochemical and DNA/BSA Binding Properties of Water-Soluble Meso-Thienyl BODIPY Derivative

rkan Karanlık [1,2], Ceren Can Karanlık [1,2], Ali Erdoğmuş [1,2]

[1] Yildiz Technical University, Department of Chemistry, Istanbul, Turkey
[2] Health Biotechnology Joint Research and Application Center of Excellence, Istanbul, Turkey

BODIPY dyes emerge as promising candidates for photosensitizers in Photodynamic Therapy (PDT) applications, revealing their potential due to the capability to produce reactive oxygen species such as singlet oxygen ($^1O_2$), a crucial element responsible for cell death in cancer and related diseases. The integration of suitable segments into the molecular structure of BODIPYs allows them to absorb within the phototherapeutic window (700–900 nm) which is very important property for PDT applications [1,2]. It has been noted that the incorporation of suitable substituents into the BODIPY core through diverse reactions has a positive impact on singlet oxygen generation. The introduction of iodine atoms or hetero-aryl segments to the BODIPY structure facilitates intersystem crossing (ISC). Similarly, the inclusion of heteroaromatic structures like thiophene or benzothiophene groups can alter both the photophysical properties of the BODIPY core and its photochemical characteristics, including singlet oxygen generation [3,4].

PDT has advantages to traditional treatment methods due to its non-invasive nature, natural selectivity, low toxicity, reusability, and rapid healing with minimal scarring. The crucial factor for singlet oxygen formation primarily relies on the choice of the photosensitizer.

Anticancer drugs target DNA intracellularly, playing a crucial role in processes like cell death, gene expression, and mutation. Consequently, DNA has emerged as a significant focus for new anticancer drugs in both pharmacological and biological contexts. Molecular targeting assumes a pivotal role in biological applications, emphasizing the significance of understanding interactions between compounds and biomolecules such as DNA, RNA, and proteins, given their binding capacities [5,6].

Within the scope of this study, the synthesis, characterization and photophysicochemical studies of water-soluble BODIPY derivative were conducted. In addition, DNA and BSA binding studies of the water-soluble BODIPY derivative were carried out.

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P118

Insight into the Mechanism of Lithium-Selenium Batteries

Tutku Mutlu-Cetinkaya [1], Rezan Demir-Cakan [1]

[1] *Gebze Technical University, Department of Chemical Engineering, Kocaeli, Turkey*

As an alternative to Lithium-Sulfur (Li-S) batteries, Lithium-Selenium (Li-Se) batteries have attracted significant attention as next generation battery systems due to the several advantages, including comparable volumetric capacity (3254 mAh/cm^3) and higher conductivity compared to Li-S batteries.[1] Nonetheless, Li-Se batteries still encounter similar challenges as Li-S batteries. The main challenges are the formation of polyselenides and their dissolution in ether-based electrolytes, namely shuttle effect, as well as the volume expansion of selenium during cycling, resulting in fast capacity decay.

Electrolyte is of great importance as it directly affects the electrochemical performance of battery, displaying different reaction pathways in different electrolytes. In general, two types of electrolytes are used in this field: ether-based and carbonate-based electrolytes. Herein, in order to investigate the impact of the electrolyte solvents, 4-electrode cycling voltammetry (CV) and 3-electrode electrochemical impedance spectroscopy (EIS), as well as ex-situ UV-vis spectroscopy were used. These analyses demonstrated that polyselenide species dissolved in ether-based electrolytes (tetraethylene glycol dimethyl ether, TEGDME) but not in carbonate-based electrolytes (ethylene carbonate/dimethyl carbonate, EC-DMC).[2] As shown in Figure 1, carbonate-based electrolytes carried out better electrochemical cyclic performance than ether-based electrolytes, which could be ascribed to the dissolution of polyselenides in TEGDME. This work indicates that carbonate-based electrolytes can be used in the field of Li-Se batteries, while Li-S batteries cannot operate in carbonate-based electrolytes due to the nucleophilic attack with carbonyl groups.

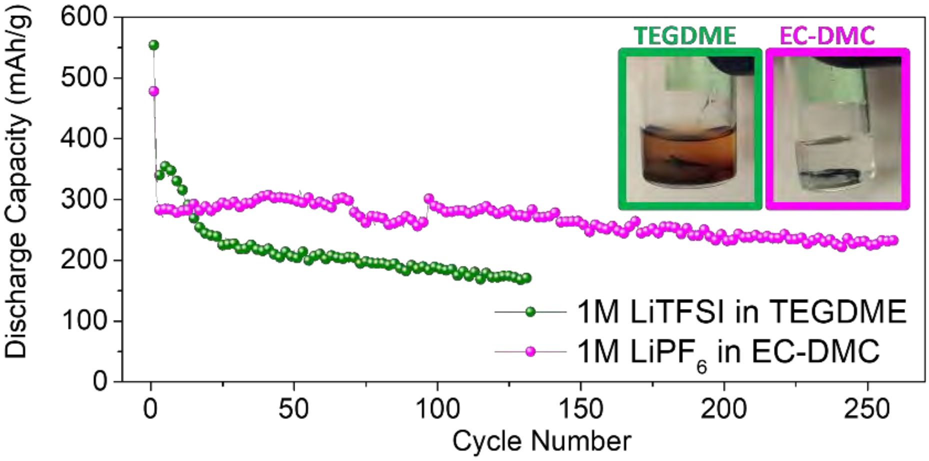

Figure 1: Cycling performance of cells in different electrolytes at 0.2 C current density. Inset: separators after the first discharge were dipped into the TEGDME and EC-DMC solvents.

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P119

Interaction of P and N species in high temperature gas phases

Mats-Ole Dewerth [1], Tina Kasper [1]

[1] *Universität Paderborn, Lehrstuhl für Technische Thermodynamik, Paderborn, Germany*

The recovery of phosphorus from biological waste streams like sewage sludge is gaining importance. As of today, a high percentage of sewage sludge in Germany is utilized in incineration plants. The importance of phosphorus and the current thermal utilization suggest a closer look at the high temperature gas phase chemistry of phosphorus. Especially the gas phase interaction of phosphorus and nitrogen species is interesting, considering the substantial concentration of both in biomass[1,2].

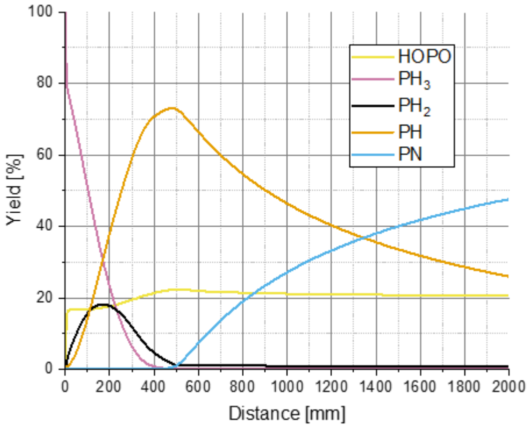

Figure 1: Yield of important P species in relation to entry concentration of PH_3

Using the plug flow reactor module of CHEMKIN, the partial oxidation of NH_3, PH_3, H_2 was simulated. O_2 and N_2O were used as oxidizing agents. Entry concentrations were 96% Ar, 1% H_2, 1.4% N_2O, 1% NH_3, 0.1% O_2 and 0.5% PH_3. A reactor length of 2000 mm, Re = 25, and a reactor diameter of 20 mm were chosen to ensure a long residence time. The main goal was to maximize the formation of phosphorus mononitride PN. High yields of up to 50% PN at the reactor outlet suggest that there is a significant interaction between phosphorus and nitrogen species, even though only two different reaction pathways were considered in the simulation.

While the simulation has yet to be validated, the high initial yield indicates that, depending on process parameters, P and N species interact in a meaningful way. Pyrolysis experiments with P and N containing flame inhibitors by Liang et al.[3] also show that PN forms in the gas phase as the dominant species. As such a closer look at the high temperature chemistry of P and N might provide new insights, that can help optimize current combustion processes of sewage sludge or even explore new synthesis pathways in the future.

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P120

Investigating the Electrochemical Battery Properties of Pillar[6]quinone: Synthesis, and DFT Study

Merve GÜNER[1], Nazmiye KILIÇ[1], Yasemin SOLMAZ[1], Selin SARIYER[2,3], Rezan DEMİR-ÇAKAN[2,3], Serkan YEŞİLOT[1]

[1] *Department of Chemistry, Gebze Technical University, Gebze, Kocaeli, Turkey*
[2] *Department of Chemical Engineering, Gebze Technical University, Gebze, Kocaeli, Turkey*
[3] *Institute of Nanotechnology, Gebze Technical University, Gebze, Kocaeli, Turkey*

Developing high-performance batteries based on organic quinone due to their high theoretical specific capacity, effective structural design is essential for nature as it paves the way for more efficient and sustainable energy storage solutions, addressing the increasing demand for clean energy, thereby mitigating environmental impact and supporting the transition towards a greener and more resilient future[1]. Pillar[6]quinone, a unique macrocyclic molecule, has emerged as a promising candidate in the realm of electrochemical energy storage, specifically in the context of rechargeable batteries[2].

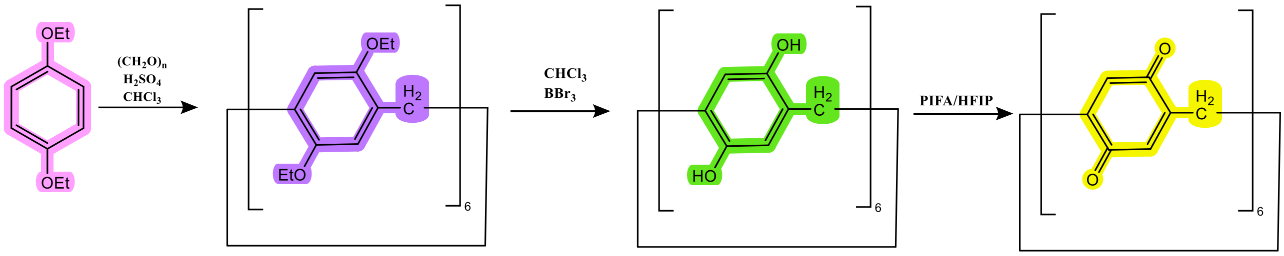

Figure 1: Synthetic pathway of pillar[6]quinone.

In this study presents a comprehensive investigation into the synthesis according to the literature[3], electrochemical properties, and density functional theory (DFT) study of pillar[6]quinone, an intriguing organic compound with a unique pillar-shaped quinone framework. These theoretical investigations provide valuable insights into the fundamental principles governing its electrochemical behavior, facilitating a deeper understanding of its redox processes, charge storage mechanisms, and overall battery performance.

We would like to thank TUBITAK for their support within the scope of 1001 - Scientific and Technological Research Projects Support Program (project no: 222Z042).

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P121

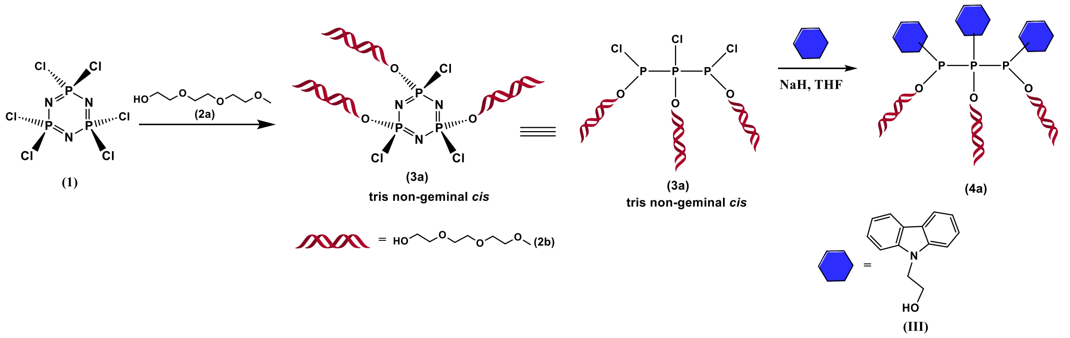
The preparation of potential anticancer agent derived from inorganic-organic hybrid molecule

Duygu Palabıyık [1], Ceylan M. Balcı [1], Serap Beşli [1]

[1] *Gebze Technical University, Faculty of Basic Sciences, Kocaeli, Turkey*

Cyclophosphazenes comprise an important class of inorganic heterocyclic compounds, having chemically stable skeletal structures and multiple reactive phosphorus chlorine units.[1] Hexachlorocyclotriphosphazene (trimer) and octachlorocyclotetraphosphazene (tetramer) are the two most accessible compounds among these series.[1] Both compounds attract the attention of researchers in synthesizing new types of compounds for targeted application areas by easily substituting with organic, inorganic, or organometallic nucleophiles.[1] As a functional group, glycol and glycol ether derivatives exhibit good solubility that makes them ideal for many applications especially biological research.[2] Also, carbazoles are prominent structures and have been widely used as an effective template in medicinal chemistry for drug discovery. Carbazole derivatives could trigger multiple cancer cell death pathways using as anticancer agents.[3]

In this work, the nucleophilic substitution reaction of hexachlorocyclotriphosphazene (**1**) with triethylene glycol monomethyl ether (**2a**) has been carried out. Thus, one side of inorganic ring was modified with hydrophilic groups that provide water solubility. After that, the obtained tris nongeminal *cis* product (**3a**) was allowed to react with *N*-ethoxycarbazole (**III**) in THF solution using NaH as base at 1:3.1 mole ratio (Scheme 1) for investigating potential anticancer characteristics of newly synthesized compound (**4a**). The target product (**4a**) was isolated and characterized by various standard techniques such as mass and elemental analyses, ^{31}P and ^{1}H NMR spectroscopies. Antitumor properties of synthesized molecule will be evaluated by in *vitro* methods using healthy colorectal pithelial cell line (CCD18Co), primary colorectal cancer cell line (Caco-2) and metastatic colorectal cancer cell line (SW620).The authors would like to thank Research University Support Program (ADEP) for financially supporting this research with grant number 2023-A-113-07.



Scheme 1: The nucleophilic substitution reactions of **1** and **3a** with **2a** and **III**, respectively.

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P122

Development and Synthesis of Artificial Nucleotide Signals to Target Immunometabolism in Plants

Julian Strippel [1], Jane E. Parker [2], Stephanie Kath-Schorr [1]

[1] University of Cologne, Institute of Organic Chemistry, Cologne, Germany
[2] Max-Planck-Institute for Plant Breeding Research, Department of Plant-Microbe-Interactions, Cologne, Germany

The use of receptors for the detection of pathogens is broadly distributed across the tree of life since a specialized immune system, consisting of innate and adaptive parts, is crucial for the survival of a species. In the last century researchers identified the Toll/interleukin-1 resistance gene (TIR) domain as an evolutionarily conserved component of both plant and ani-mal immune systems.[1] TIR enzymes consume nicotinamide adenine dinucleotide (NAD+) and produce crucial immuno-metabolites. While the depletion of NAD+ can also trigger down-stream signalling, the metabolites play a crucial role in the immune response by activating specific enzyme complexes.[1]

While most of these downstream pathways are yet not fully understood, in 2022 the Parker group identified two pairs of immuno-metabolites in plants, which are recognized by a family of lipase-like proteins consisting of Enhanced Disease Susceptibility 1 (EDS1) domains and its exclusive partners, the Phytoalexin Deficient 4 (PAD4) domain and the Senescence Associated Gene 101 (SAG101) domain.[2] Association of the signalling molecule with the EDS1 complex leads to a conformational change in the PAD4/SAG101 domain which promotes their association with a co-functioning intracellular nucleotide-binding leucine-rich repeat (NLR) receptor to induce pathogen resistance.[2] Specific activation of these EDS1 enzyme complexes lays the foundation for an applied crop protection strategy. Our aim is to develop synthetic analogues of the naturally occurring signal molecules that exhibit improved biological properties.

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P123a

Promovieren und forschen in Jena

Leanne M. Stafast[1], Vivien Sulimma[1], Claudia Hilbert[1]

[1] Chemisch-Geowissenschaftliche Fakultät, Friedrich-Schiller-Universität, Jena, Deutschland

Schon im 19. Jahrhundert war bekannt „[...] in Jene lebt sich's bene",[1] und es ist auch heute noch so. Einmal von der Autobahn in die Stadt gelangt, lässt sie einen nicht mehr los, insbesondere wenn es um Promotionsoptionen geht. An der Friedrich-Schiller-Universität Jena gibt es unter anderem die Möglichkeit, im Rahmen einer der zahlreichen, häufig international ausgerichteten Drittmittelprojekte oder der rund 20 Graduiertenschulen und Graduiertenkollegs zu promovieren. Im naturwissenschaftlichen Bereich und insbesondere in der Chemie sind unter anderem das Exzellencluster „Balance of the Microverse" und die Sonderforschungsbereiche „PolyTarget" und „CataLight" zu nennen. Hinzu kommt die Möglichkeit, eine Promotion in Kooperation mit einer anderen Einrichtung durchzuführen. Hier stehen in Jena zahlreiche außeruniversitäre und renommierte Forschungsinstitute zur Verfügung, wie etwa mehrere Max-Planck-Institute und Institute der Leibniz-Gemeinschaft. Die engen Kooperationen zwischen der Universität Jena, den außeruniversitären Forschungseinrichtungen und der regionalen Wirtschaft umspannt einen breiten Rahmen aktueller Forschungsthemen.

Zur exzellenten Forschungsinfrastruktur in Jena gehören mehrere moderne Forschungsgebäude, nicht nur am Beutenberg Campus im Süden der Stadt, sondern auch zentral gelegen in der Innenstadt. Zu nennen ist beispielsweise das neu errichtete Center for Energy and Environmental Chemistry II, welches unter anderem das 2023 gegründete Helmholtz-Institut für Polymere in Energieanwendungen Jena beherbergt. [6]

Egal ob im Bereich Mikrobiologie, Chemische Biologie, Infektionsbiologie, Medizin, Ökologie, Optik/Photonik, Materialwissenschaften oder Bioinformatik – für jeden ist etwas dabei, sei es eine Promotion oder eine Postdoc-Position. Die Graduierten-Akademie[7] unterstützt Promovierende und Postdocs auf ihrem Karriereweg, unter anderem durch Qualifizierungsprogramme und als Dacheinrichtung der strukturierten Promotionsprogramme innerhalb von Graduiertenschulen und Graduiertenkollegs.

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P123b

Chemie studieren in Jena

Leanne M. Stafast[1], Sabrina Even[1], Claudia Hilbert[1]

[1] Friedrich-Schiller-Universität Jena, Chemisch-Geowissenschaftliche Fakultät, Jena, Deutschland

In Jena, berühmt für Otto Schott und Carl Zeiss sowie den legendären Spaziergang von Goethe und Schiller, der den Grundstein für ihre Freundschaft legte, gibt es nicht nur für Geschichtsenthusiasten zahlreiche faszinierende Orte zu entdecken. Auch für alle naturwissenschaftlich Begeisterten ist Jena die ideale Stadt. Aber was macht Jena und vor allem die Friedrich-Schiller-Universität (FSU) so besonders, dass man einfach nicht widerstehen kann, nach Thüringen zu ziehen? Neben zahlreichen außeruniversitären Forschungseinrichtungen und High-Tech-Unternehmen, die die Möglichkeit bieten auch nach dem Studium der Forschung treu zu bleiben oder einen attraktiven Arbeitsplatz zu finden, kann Jena auch mit einem reichhaltigen kulturellen Angebot, einer wunderbaren Landschaft und zahlreichen seltenen Orchideenarten im Frühjahr bezaubern. Kurz gesagt: In Jena ist „das Paradies“.[1]

Die Chemisch-Geowissenschaftliche Fakultät bietet ein vielfältiges Studienangebot, darunter Bachelor- und Lehramtsstudiengänge in Chemie sowie vier Masterstudiengänge, Chemie, Chemische Biologie, Chemie - Energie – Umwelt und der englischsprachige Studiengang „Chemistry of Materials“. Insbesondere die drei letztgenannten Studiengänge sind stark interdisziplinär ausgerichtet. Sie sind ein kooperatives Studienangebot der Chemisch-Geowissenschaftlichen Fakultät mit weiteren Fakultäten der FSU Jena. Die Zusammenarbeit mit der Physikalisch-Astronomischen Fakultät ermöglicht zudem interdisziplinäre Studienmöglichkeiten im Bereich Werkstoffwissenschaften und Medical Photonics.[2] Außerdem profitieren weitere Studiengänge von dem guten chemischen Lehrangebot, wie etwa im Bereich Geowissenschaften. Insgesamt bietet die Fakultät eine breite Palette von Studienmöglichkeiten und es zeigt sich eins: Interdisziplinarität wird bei uns großgeschrieben.

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P123c

Die Geschichte der Chemie in Jena

Synnöve Lemke[1], Verena Müller[1], Gustav Döhring[1]

[1] *Friedrich-Schiller-Universität Jena, Jena, Deutschland*

Die Geschichte der Chemie in Jena erstreckt sich bereits über 450 Jahre. Von Werner Rolfinks über Johann Friedrich Döbereiner bis hin zu Otto Schott. Sie alle prägten die Friedrich-Schiller-Universität Jena nachhaltig im Fachbereich der Chemie. Schon früh war klar: In Jena stimmt die Chemie.

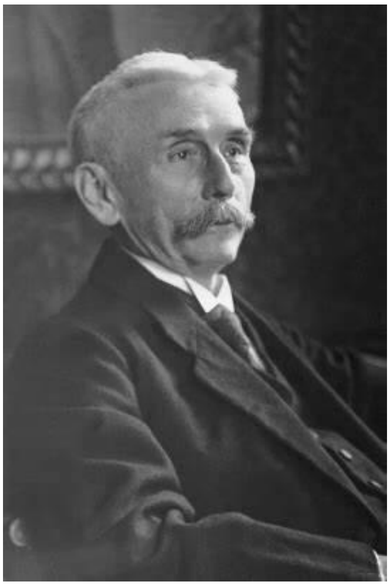

Abbildung 1: Otto Schott[2]

Abbildung 2: Johann Friedrich Döbereiner[4]

Die revolutionäre Ernennung Johann Friedrich August Göttling 1789 zum ersten deutschen extraordinären Professor für Chemie in Jena schlug starke Wellen. Bis dato wurde die Chemie in Deutschland nur „nebenbei“ von der medizinischen Fakultät mitvertreten. Sein Nachfolger Johann Friedrich Döbereiner (Abbildung 2) schaffte es sogar mit staatlicher Unterstützung aus Weimar 1810 ein chemisches Institut in Jena zu errichten und mithilfe von Goethe private Geldgeber für die kostspielige Ausrüstung zu finden.[1]

1875 promovierte Otto Schott (Abbildung 1) in Jena im Fachgebiet der Glaschemie und entwickelte das revolutionäre Lithiumglas. Durch Schott konnten nun erstmals Gläser mit exakt vorherbestimmbaren und reproduzierbaren Eigenschaften für optische Anwendungen hergestellt werden.[2,3]

Mit diesem kleinen historischen Abriss möchten wir einige bedeutsame Chemiker Jenas vorstellen und ihr Lebenswerk ehren.

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P123d

Das JCF Jena

Leanne M. Stafast [1], Paul Pfeiffer[1], Synnöve Lemke[1], Verena Müller[1]

[1] *Chemisch-Geowissenschaftliche Fakultät, Friedrich-Schiller-Universität, Jena, Deutschland*

Jena, zentral im Herzen Deutschlands gelegen, wird von Muschelkalkhängen entlang der Saale umrahmt. Die Stadt beherbergt zahlreiche Forschungseinrichtungen wie z.B: drei Max-Planck-Institute, das Fraunhofer-Institut für Angewandte Optik und Feinmechanik, drei Leibniz Institute und zwei Helmholtz-Institute.[1-2] In Jena haben sich im Laufe der Zeit bedeutende Unternehmen angesiedelt, und die Stadt hat im Laufe der Jahre schon viele berühmte Persönlichkeiten beherbergt, darunter Ricarda Huch, Otto Schott und Johann Wolfgang Döbereiner.[3]

Das JungChemikerForum Jena besteht derzeit aus Studierenden in verschiedenen Stadien – Bachelor, Master und Promotion. Diese Vielfalt unserer Mitglieder spiegelt sich auch in unseren Veranstaltungen wider.

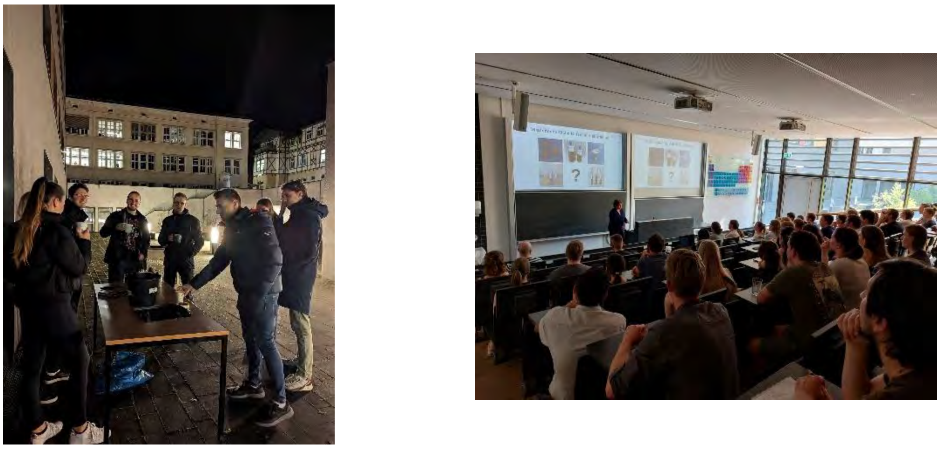

Bild 1: Impressionen unserer Veranstaltungen (links “Triff den Prof!“, rechts: Vortrag mit Dr. Theofel).

Unsere monatlichen Stammtische bieten die Möglichkeit, sich auszutauschen, Ideen zu besprechen und insbesondere die Projekte für das laufende Semester zu planen. Von wissenschaftlichen Vorträgen über Schnitzeljagden, Wanderungen und Exkursionen zu umliegenden Firmen bis hin zur Vorstellung von Dozenten an unserer Universität ist für jeden etwas dabei. Ganz neu dabei sind auch Workshops zum Thema mentale Gesundheit.

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P124

Photosensitizer Candidate New Water-Soluble BODIPYs: Synthesis and Properties

Seda Cetindere [1], Perihan Kızılkaya [1, 2]

[1] Gebze Technical University, Department of Chemistry, Kocaeli, Türkiye
[2] Trakya University, Department of Chemistry, Edirne, Türkiye

Cancer, which is accepted as the disease of our age due to the increasing number of cases in recent years, is a disease caused by tumours that arise as a result of uncontrolled division and proliferation of cells in an organ or tissue. Although many different methods are used to combat this extremely deadly disease, no definitive treatment has yet been found. For this reason, research on cancer treatment continues intensively. It is known that the treatment methods that are effective especially in early diagnosis are chemotherapy, radiotherapy and surgical intervention. In addition to these treatment methods, alternative treatment methods are also being developed and used [1]. Photodynamic therapy (PDT) is an alternative non-surgical method for cancer treatment, since the side effects are few, the cells do not develop resistance to the drug, and the drug can be given to the patient at low doses [2]. Boron-dipyrromethene (BODIPY) based photosensitizers, have in means of unique photophysical properties, are useful in PDT method [3]. Recent studies in BODIPY based molecular therapeutics allow the development of treatment with highly tumour selectivity in PDT method [4]. Within the scope of this study, it is aimed to design, synthesis, and properties of new water-soluble BODIPY compounds (**1** and **2**), which have potential using in cancer treatment with PDT.

Acknowledgement: We would like to thank GTUBAP (Project No: 2022-A-105-43) for financial support for this work.

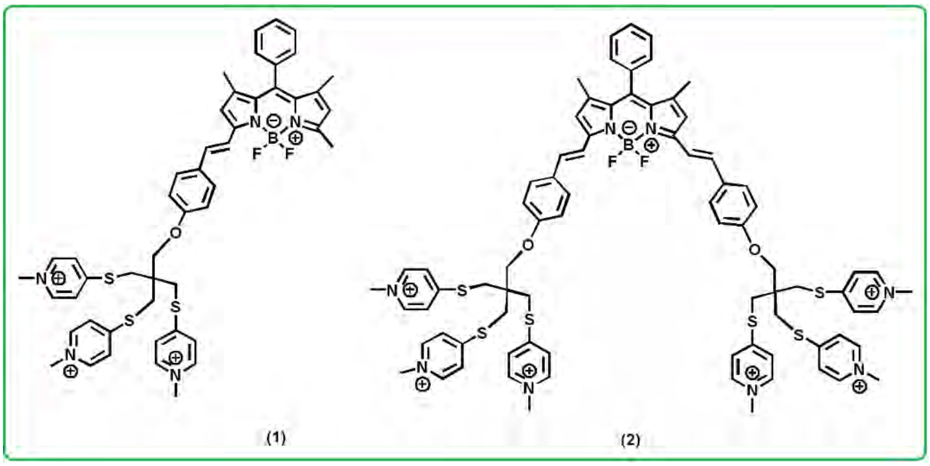

Figure 1: Water soluble BODIPY compounds.

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P125

Ligand Design in the Direct Asymmetric Reductive Amination

Maximilian Menche [1,2]

[1] BASF SE, Quantum Chemistry, Ludwigshafen, Germany
[2] Catalysis Research Laboratory (CaRLa), Heidelberg, Germany

The asymmetric ruthenium-catalysed reductive amination employing ammonia and hydrogen to primary amines is a promising access to important chiral building blocks. After we demonstrated the capability of our catalyst to perform the chemo- and enantioselective reaction while using simple ammonia gas as a reagent, one of the most attractive and industrially relevant nitrogen sources, the mechanism of this reaction was investigated by means of density functional theory. We found a viable pathway, which explains the observed trends and magnitude of enantioselectivity through the halide series in good agreement with the experimental data. The in-depth investigation of substrate conformers during the reaction turned out to be crucial in obtaining an accurate prediction for the enantioselectivity.[1] Subsequently, a predictive model based on the ligand bite angle was developed to allow for a big data approach in screening different ligands. A selected set of ligands was tested and validated with DFT calculations and experiments, which revealed a variety of difficulties and drawbacks of such approaches. The examples strongly support our believes that computations and experiments work best and most effectively hand-in-hand with constant exchange and guided our next steps in enantioselectivity prediction to be more effective.[2]

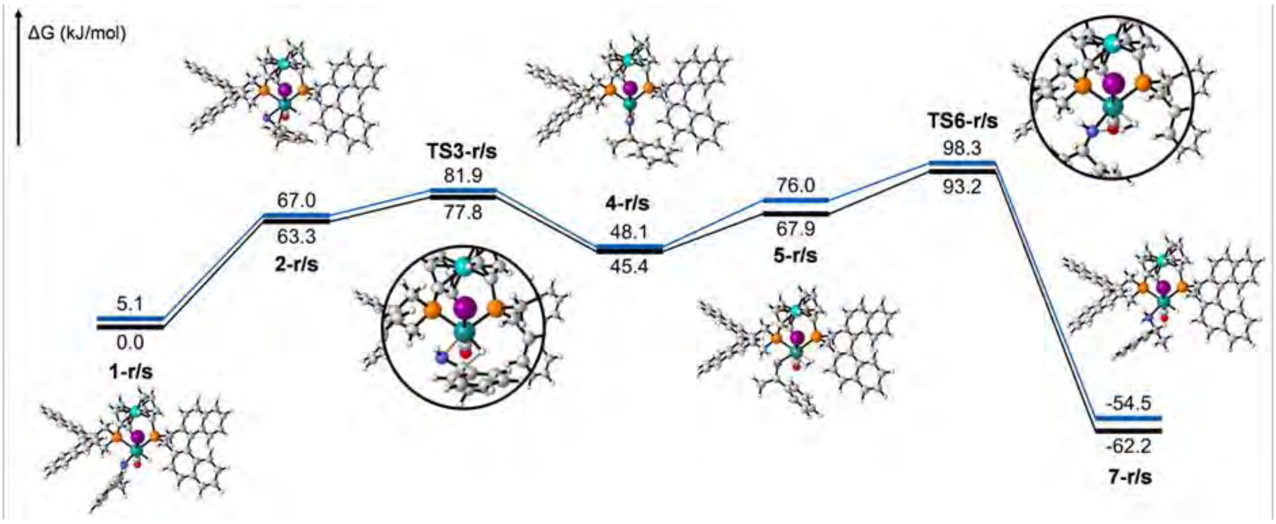

Figure 1: Computed mechanism for the asymmetric Ru-catalysed reductive amination with NH_3 and H_2.

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P126

Investigation of the interactions between cationic guar gum and the biosurfactant rhamnolipid

Jörn Phillipp Optatzi[1,2], Peter Schmiedel[1], Birgit Glüsen[2]

[1] LRR-Physical Chemistry, Henkel AG & Co. KGaA, 40589 Düsseldorf, Germany
[2] TH Köln – University of Applied Sciences, 51368 Leverkusen, Germany

Combinations of anionic surfactants and cationic polyelectrolytes are commonly used as ingredients in several different applications. In shampoos, for instance, they help to reduce the combing force of the hair and they impart a smooth hair feeling. Laundry and cleaning applications contain in most cases ionic surfactants or surfactant mixtures and can also comprise polyelectrolytes. In this case the polyelectrolytes can act as soil release polymers and prevent re-soiling.

The bulk interactions of mixtures of polymers and surfactants are decisively controlling the adsorption behavior of the polyelectrolytes onto substrates. These have been intensively investigated since the 50's years of the 20th century.[1–3] However, in view of climate change, a reduction of the emission of greenhouse gases is necessary. Additionally, the mostly poor biodegradability of the used polymers leads to environmental pollution. Therefore, it is necessary to replace these complex, well-established systems by green and sustainable polymer-surfactant systems. Conventional systems, containing a poly-cation and anionic surfactants, are well studied.[4–6] Recent studies mostly investigate systems containing either a (well described) biosurfactant, or a (well described) biopolymer. There is, however, still a lack of studies dealing with combinations of both biopolymers and biosurfactants.

In this work, we investigate the bulk interaction behavior of the bio-based cationic polymer guar hydroxypropyltrimonium chloride and the biosurfactant rhamnolipid using among others light scattering methods (DLS, DLS-based microrheology). Adsorption properties onto model surfaces were studied using quartz crystal microbalance with dissipation (QCM-D). Modified gold surfaces imitating negatively charged damaged hair were used. By an adjustment of the interaction properties in bulk, a significant enhancement of the polymer deposition onto the model surfaces in comparison to pure polymer solution was observable.

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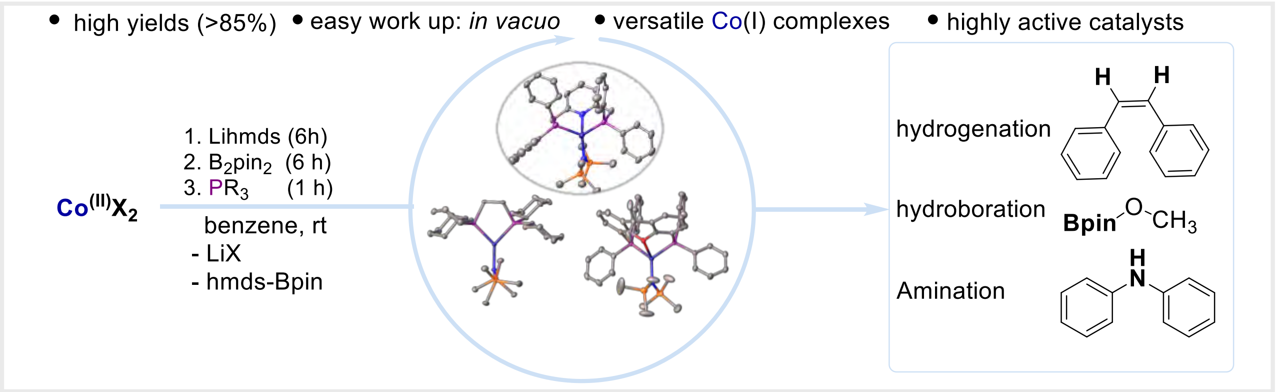
P127

A convenient synthesis of Co(I) complexes and their applications

Lea Luxenberger[1], Axel Jacobi von Wangelin[1]

[1]*Institute of inorganic and applied science, University Hamburg, Hamburg, Germany*

Increasing energy consumption, the scarcity of fossil resources highlight the necessity for 3d metals in catalysis. Cobalt, sharing electronic similarities with widely used iridium, palladium, and ruthenium catalysts, emerges as a highly suitable metal center for catalyst development.[1] Notably, Cobalt has recently gained prominence in crucial reactions within pharmaceutical syntheses, including cross-coupling reactions, hydroboration, and hydrogenation, as evidenced by several research groups.[1-3] Of particular interest is cobalt in the oxidation state 1, owing to the significant C-H activation processes involving Co(I)-Co(III) redox processes akin to the well-known Ir(III)-Ir(V) pathways.[4] The preparation of ligand-stabilized cobalt(I) has mostly been performed by sequential ligand exchange and reduction steps starting from available cobalt(II) salt precursors.[3-4] In this study, we present a highly effective, high-yielding, and versatile strategy employing the readily available precursor $Co[N(SiMe_3)_2]_2$, $Co(hmds)_2$ along with the commercial borane reagent bis(pinacolato)diboron, B_2pin_2, in the presence of diverse phosphine ligands. This approach leverages two distinct properties for rapid conversion: *i)* the high driving force of N-B Lewis pairing and ii) the intrinsic reducing power of the B-B bond induces Co(II)→Co(I) reduction. The resultant cobalt(I) phosphine complexes can be obtained with different coordination patterns including monodentate, chelating, and pincer-type phosphines. The amido ligand imparts basic reactivity to the complex, which can be harnessed in the initial activation of substrates. The catalytic efficacy of these complexes has been successfully demonstrated.



Scheme 1: New B_2pin_2-mediated ligand substitution and reduction pathway. Showcasing selected applications of such prepared cobalt(I) complexes in catalytic hydroboration, hydrogenation, and amination.

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P128

Luminescent Cadmium- and Lead-free Core/Shell Quantum Dots for optoelectronic Applications in the Near-Infrared Range

Ekaterina Salikhova [1,2], Tobias Jochum [1], Hendrik Schlicke [3], Sören Becker [1], Alf Mews [2], Jan Niehaus [1]

[1] Fraunhofer IAP-CAN, Hamburg, Germany
[2] University of Hamburg, Hamburg, Germany
[3] Leibniz-Institut für Polymerforschung, Dresden, Germany

Luminescent Quantum Dots (QDs) with a near-infrared (NIR) band gap are attractive for applications such as quantum light emitting diodes, security and bioimaging. Especially for the biomedical applications, and due to environmental concerns, the development of cadmium- and lead-free core/shell QDs with effective surface passivation is required.[1,2]

However, when compared to other semiconductor nanoparticles, the wet-chemical synthesis of RoHS-compliant III-V and I-III-VI systems is significally less investigated. The stronger covalent character of III-V material bonding requires harsher reaction conditions and makes size and size distribution control more difficult. The most developed synthesis routes for InAs rely on pyrophoric, toxic, and not commercially available arsenic precursors.[1] For I-III-V systems like CuInS(Se), it is difficult to control simultaneously the reactivity of multiple precursors during the synthesis without using a sequential cation exchange method.[2]

Here we will present three RoHS-compliant core/shell QD systems for optoelectronic applications. These are InAs/ZnS, InAs/ZnSe/ZnS and CISe/CIS. The QDs are synthesized either via a *hot injection* method or via a template-based approach using CdSe/CdS. The absence of Cadmium was verified by energy dispersive X-ray spectroscopy. The optical properties of the produced QDs are going to be discussed.

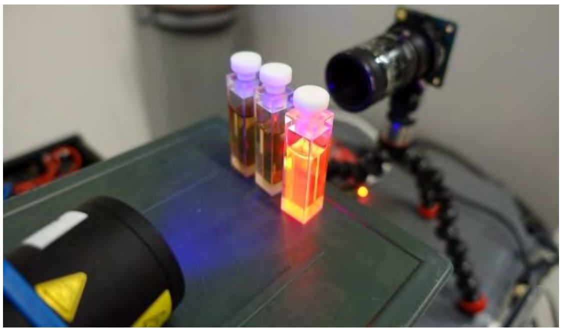

Figure 1: Different QD solutions under UV excitation imaged using a regular camera.

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P129

Supercapacitor properties of boron carbon nitride-filled PPy/PLA ternary nanocomposites

Melike Yıldız[1], Hüsnü Cankurtaran[1], Volkan Uğraşkan[1]

[1] *Yıldız Technical University, Department of Chemistry, 34220 Esenler, İstanbu rkiye*

Metal-free B, N, S and P-doped carbon-based 2D materials is of great importance for technological areas such as new energy storage systems, smart sensors, rapid and effective environmental remediation of hazardous chemicals or synthesis of various compounds by catalytic reactions[1]. Conductive polymer composites of such materials have attracted a great deal of attention in the field of supercapacitors in recent years[2]. 2D materials can provide not only electrical double-layer capacitance by ion adsorption/desorption, but also pseudo-capacitance by redox reaction. Besides, large surface of 2D materials provides excellent conductivity for fast electron transfer. Furthermore, the intermolecular binding between 2D material and conductive polymer particles contributes to the structural stability of the components[3].

In this study, boron carbon nitride (BCN)-filled polypyrrole/polylactic acid (PPy/PLA) ternary composites were synthesized. These composites were characterized by SEM, XRD, BET and FTIR measurements. The electrochemical behavior and capacitive performance of the thin films of these materials were evaluated by CV, GCD and impedance measurements. Some performance properties of the thin film capacitors, such as specific capacitance, power/energy density, cycling stability and self-decharge, were investigated. It was confirmed that the BCN has a synergistic effect on the capacitive performance of the composite films. As a result, PPy/PLA/BCN ternary composites have been shown to be good candidates for high-performance supercapacitors.

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P130

From tissue to single-cell MALDI-MS imaging

Felix-Levin Hormann [1,2], Sven Heiles [1,2]

[1] *Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany*
[2] *University of Duisburg-Essen, Faculty of Chemistry, Essen, Germany*

Scientist are faced with two options analyzing biological tissue: spatially resolved but targeted analysis using methods such as fluorescence microscopy, or untargeted analysis using e.g., mass spectrometry (MS), sacrificing spatial information. MS imaging (MSI) methods such as matrix-assisted laser desorption/ionization (MALDI)-MSI bridge this gap and allows researchers to spatially resolve the distribution of biomolecules and gain information about the molecular markup of tissues.

In MALDI-MSI a focused laser beam is scanned across a matrix covered tissue in a grid like fashion. For each sampling spot a mass spectrum and the corresponding location are recorded. By selecting specific mass-over-charge (*m*/*z*) features and plotting their intensity for each pixel an ion intensity distribution as shown in Figure 1, is obtained. This procedure can be repeated for all detected *m*/*z*-signals. Our group focuses on improving data quality, reproducibility, and lateral resolution for MALDI-MSI – tackling all steps in the analysis workflow from sample pre-treatment and instrumentation to data analysis.

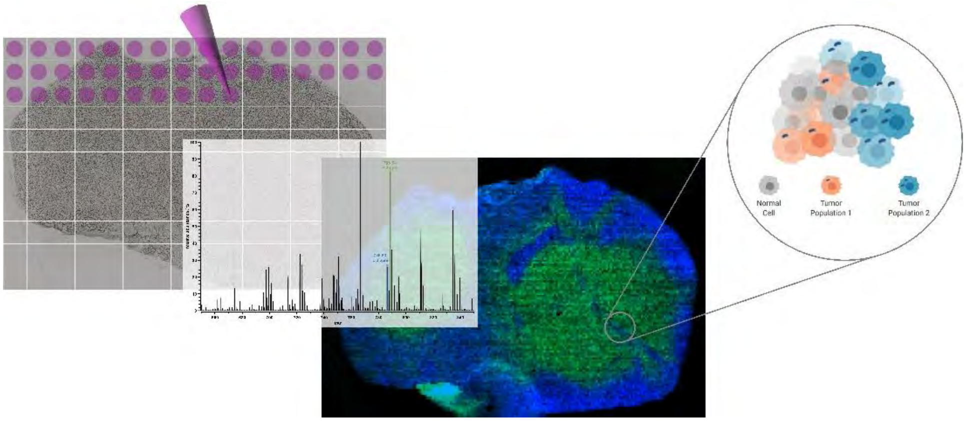

Figure 1: General principal of MALDI-MSI and heterogeneity of tissue on a subcellular scale.[1]

Diseases like cancer or myocardial infarcts lead to confined heterogeneous molecular signatures within the tissue.[1] As these areas might be as small as few cells, we aim to routinely analyze single cells in tissue. Prior to that, we are optimizing our sample preparation and analysis workflows on cell cultures to proof the required lateral resolution and signal coverage revealing molecular cell-to-cell differences as previously demonstrated for microglia cells.[2] As a proof of concept, we show an example from O2-US(FUCCI4) cells, which are genetically modified to have unique fluorescence readouts based on their cell cycle state.[3] Our method allows us to analyze the lipidome of single cells and correlate it accordingly to the cell cycle state combining fluorescence microscopy and MALDI-MSI demonstrating its applicability in the in-depth characterization of cellular lipidome.

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P131

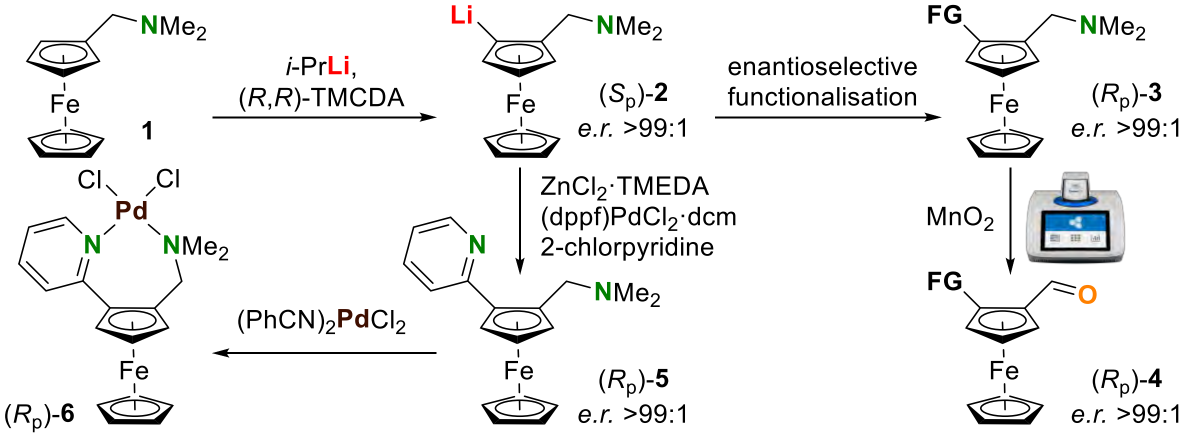
Planar chiral ferrocenes as key compounds for asymmetrically controlled processes

Paul E. Schneider[1], Carsten Strohmann[1]

[1] *TU Dortmund University, Faculty of Chemistry and Chemical Biology, Dortmund, Germany*

Planar chiral ferrocenes are often used as a chiral backbone for asymmetric ligands suitable for asymmetric catalysis.[1] In general, synthetic strategies for planar chiral ferrocene ligands such as Josiphos are based on expensive enantiomerically enriched educts like Ugi´s amine.[2] This leads us to the challenge of providing facile access to planar chiral ferrocenes as key building blocks for inexpensive asymmetric ligands.

We were able to face this challenge by the stereoselective *ortho*-lithiation of *N,N*-dimethylaminomethylferrocene (**1**) with *i*-propyllithium and the chiral ligand (*R*,*R*)-TMCDA. The reaction led to *e.r.* up to >99:1 and was also possible with catalytic amounts of TMCDA.[3] We utilised this defined enantiopure lithium aggregate (*S*p)-**2** for the enantioselective one-pot *ortho*-functionalisation, with various functional groups [**FG** e.g. pyridinyl substituent (*R*p)-**5**] and following transition metal complexations [e.g. (*R*p)-**6**].



Scheme 1: Overview of the discussed synthetic procedures.

We also could transform the *N,N*-dimethylaminomethylgroup in an aldehyde through a newly developed microwave synthesis, which tolerated various functional groups. This two-step asymmetric synthesis with catalytic amounts of the chiral ligand led to ortho-substituted ferrocenealdehydes [(Rp)-**4**]. This is an alternative to Kagan's chiral acetal method taking five synthesis steps and requiring stoichiometric amounts of a chiral auxiliary.[4]

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P132

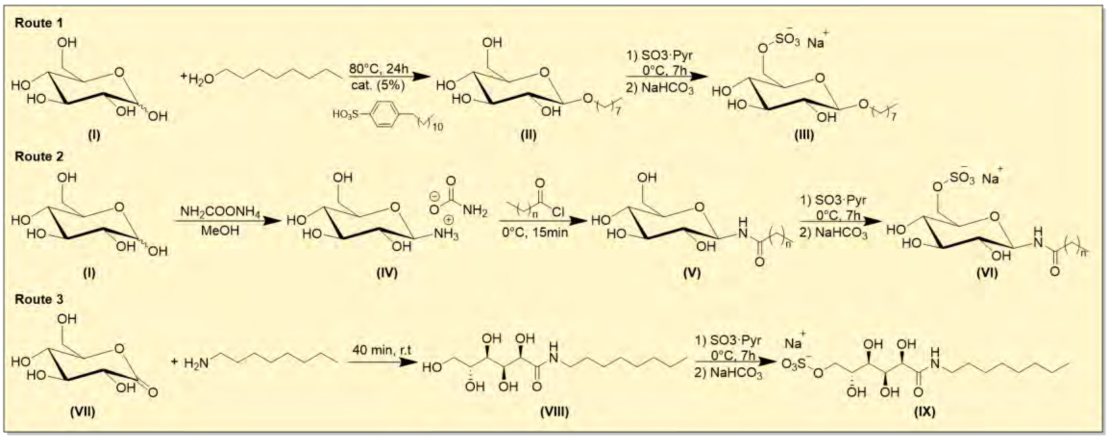
Anionic Sugar-Based Surfactants for low temperature Detergency

Philipp Effnert [1], Dr. S. Lindhoud [1], Prof. Dr. J. Lange [1], Prof. Dr. J. Huskens [1]

[1] *Twente University, Molecular Nanofabrication, Enschede, Netherlands*

During the last five years, the impact of surfactants in our everyday lives has increased continuously. Most commonly, surfactants are used for detergency. During the COVID-19 pandemic, they were used excessively for cleaning surfaces or disinfecting hands. Because of the big demand for surfactants, the industry produced well over 15 million tons of surfactants while the demand is still increasing.[1] In the past, surfactants were produced from crude oil. Due to the climate change and the shortage of oil, next-generation surfactants must be developed. They must fulfil criteria such as coming from a renewable restock, low toxicity, and biodegradability. That’s why green surfactants have become more popular in recent years.[1,2]

Understanding the chemical structure is important for rationally designing new surfactants.[1,3] Therefore, different Sugar-Based Surfactants(SBS)-derivatives must be synthesized.[4] Depending on the structural elements such as linker group, stereo-/ regio-chemistry the physiochemical properties can be modified for the respective application. In this project the SBS shall be implemented in room temperature detergency.



Scheme 1: The scheme outlines three routes for Sugar-based Surfactant (SBS) synthesis. Route 1, the common approach, employs an ether linker. Route 2 incorporates a peptide bond, introducing unique chemical features. Route 3 yields an acyclic derivative, offering molecular flexibility. These diverse routes enable precise control over SBS structure and properties for tailored applications.

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P133

Synergisms of enzyme-additive mixtures for solid fat removal

Christoph Bayer [1], Mathias Ulbricht [1], Karlheinz Graf [2], Arnd Kessler [3]

[1] University of Duisburg-Essen, Institute of Technical Chemistry, Essen, Germany
[2] Hochschule Niederrhein, Institute of Physical Chemistry, Krefeld, Germany
[3] Henkel AG & Co. KGaA, GRR Smart Washing Technology, Düsseldorf, Germany

Solid fats are removed in a standard household dishwasher by the interaction of mechanics, temperature, chemistry and time. A solid fat is melted by high temperatures (T > 50°C) and removed mechanically over time from the dish surfaces with the help of chemical components such as surfactants.[1,2] If high temperatures are missing, such as in newly developed low-temperature dishwashing programs (T < 30°C), then the process for solid fat removal must be adapted.[3] In this work, this is done by the enzyme-catalyzed fat hydrolysis known from the literature.[4] Investigations using the quartz crystal microbalance with dissipation monitoring showed that the enzyme-catalyzed removal of a solid crystalline fat is a desorption process which can be described in a good approximation by the Sauerbrey equation. For this process, a desorption or reaction time can be defined and subsequently determined for different chemical systems. A comparison of the reaction times for these systems revealed that the enzyme-catalyzed fat removal can be accelerated by the addition of sustainable additives. Furthermore, the process parameters play a decisive role. Taking these factors into account, this work presents a chemical system that can remove solid fats at low temperatures in a time-efficient and sustainable manner for dishwashing applications.

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P134

Enhanced photoelectrocatalytic degradation of methylene blue using Li-doped ERGO/TiO_2 nanocomposite photoanode under visible light

Zeynep Selin Başaran Yılmaz [1], Ümit Demir [1]

[1] *Gebze Technical University, Department of Chemistry, Kocaeli, Turkey*

In recent years, industrial process-generated pollutants in wastewater threaten both environmental ecology and human health, notably from complex compounds like endocrine disruptors and dyes such as methylene blue. Conventional methods used to treat methylene blue in wastewater lack energy efficiency and produce additional pollutants. While photocatalysis offers an alternative, its drawback lies in the continuous mixing and filtration requirements for the photocatalyst, limiting its cost-effectiveness and broad application. Recently, photoelectrocatalysis (PEC) has emerged as a promising technology, combining photocatalysis and electrochemistry, offering efficient methylene blue removal from aqueous solutions.[1] In this study, the aim was to fabricate a photoanode based on Li-doped TiO_2 decorated with an electrochemically reduced graphene oxide (ERGO) nanocomposite, capable of operating across the entire spectrum of sunlight without the need for applied voltage, to achieve effective photoelectrocatalytic degradation of methylene blue. ERGO/TiO_2 nanocomposite was prepared on FTO by co-electrodeposition technique which is a simple, cheap and eco-friendly. ERGO/TiO_2 photoelectrodes were doped by electrochemically reductive self-doping from aqueous medium containing Li^+ cations to form Ti^{3+} defects and O vacancies in the nanostructure.[2] Li-ERGO/TiO_2 photoanode were characterized by XRD, XPS, and FESEM techniques. The PEC degradation was carried out in a quartz cell containing MB and Na_2SO_4 solution with 2-electrodes, Li-ERGO/TiO_2 and platinum wire were used as photoanode and cathode, respectively. The cell was illuminated by using a solar simulator without an applied voltage. The degradation of the MB solution was monitored using a UV-Vis spectrophotometer. Li-ERGO/TiO_2 photoanode exhibited 98% PEC degradation of MB over a duration of 210 minutes.

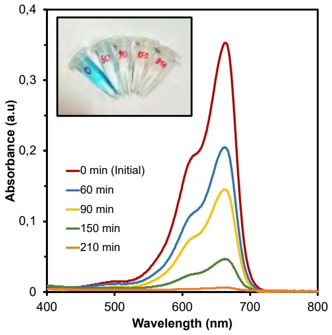

Figure 1: Time-dependent UV-visible absorption spectra for PEC degradation of methylene blue

The Scientific and Technological Research Council of Turkey (TUBITAK) is gratefully acknowledged for the funding of these works (Project no.122Z028).

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P135a

Automated Quantum Chemical Microsolvation in Arbitrary Solvents

Lukas Magenheim[1], Radu A. Talmazan[1] and Maren Podewitz[1]

[1] *Technische Universität Wien, Institut für Materialchemie, Vienna, Austria*

Molecules in solution, typically denoted as solutes, are surrounded by solvent molecules with which they interact. These interactions have a direct influence on the properties and reactivity of the solute at hand. To obtain a more accurate chemical model, as well as improve the description of the system behaviour, it is vital that solvent effects are taken into account.

In quantum chemical descriptions, those solvent effects are either treated implicitly, accounting for bulk properties only – in its simplest way by an electrical permittivity – or explicitly, by defining an arbitrary number of solvent molecules around the solute. This approach poses two questions:

- Where and how should those solvents be placed?
- How many are needed to capture most of the relevant interactions while minimizing the computational workload?

In a previous work,[1] we devised a protocol for systems solvated in water that extracts energetic and entropic information from MD simulation derived data. This protocol makes use of the Grid Imhomogenous Solvation Theory (GIST)[2] to determine solute-solvent interaction on a grid. Here, we present the completely revised and extended protocol, which is now fit to evaluate favorable solvation sites for a larger set of rigid solvents, such as dichloromethane or DMSO.[3] We showcased the applicability of our methodology at several examples ranging from solvatochromic substances to transition-metal containing bioinorganic compounds such as Vitamin B_{12}.

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P135b

Austrian Young Chemists Network

Lukas Magenheim [1], Leonhard Hecht [1], Sarah Keck [1], Jakob Ehrenbrandtner [1]

[1] *Österreichische Chemische Gesellschaft, Junge Chemie Österreich, Austria*

The Austrian Young Chemists Network is a subdivision of the Austrian Chemical Society. We aim to bring the next generation of chemists closer together and connect them with educational institutions and partners in business on both the national and international level.

Over the past ten years, more than 90 motivated students have successfully built up our national network comprising five regional representations in Innsbruck, Salzburg, Linz, Vienna, and Graz. More than 150 events, ranging from specialist lectures, workshops, excursions to internal and external university partners, and networking events for students, have been very well received by students and interested parties throughout Austria.

Furthermore, the Austrian Young Chemists Network is part of the European Young Chemists Network (EYCN) and the International Young Chemists Network (IYCN).

Here, we present our network and our activities.

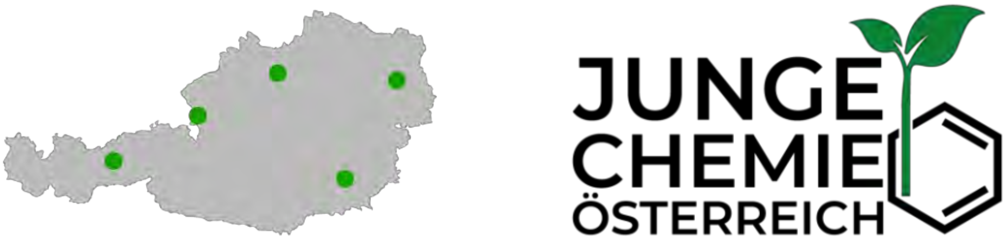

Figure 1: The Austrian Young Chemists Network

P136

The role of nonsecular terms in vibrational polaritons

R. Kevin Kessing [1], Marcos S. Tacca [1], James Lim [1], Susana F. Huelga [1], Martin B. Plenio [1]

[1] *Ulm University, Institute of Theoretical Physics, Ulm, Germany*

Recent advances in strongly coupling infrared electromagnetic modes to molecular vibrations in resonator cavities have spurred interest in polaritonic systems and opened up new avenues of research such as polaritonic chemistry, in which the strong light-matter coupling and potentially hybridized nature of the system's eigenstates serve to modify chemical reactivity.

To thoroughly comprehend the underlying mechanisms, and, furthermore, to establish optimal methods of harnessing and steering such a light-induced control of chemistry, it is imperative to establish a theoretical framework in which the essential features and mechanisms of said polaritonic chemistry can be identified.

In the theoretical modeling of strongly coupled light-matter systems, dipole coupling between the electromagnetic mode and the molecular modes is typically assumed $(H_{\text{int}} \propto \vec{\mu} \cdot \vec{d})$, which can ultimately be in the terms

$$(a^\dagger + a)(b^\dagger + b) = a^\dagger b + b^\dagger a + a^\dagger b^\dagger + ab, \tag{1}$$

where $a, a^\dagger$ and $b, b^\dagger$ are the annihilation/creation operators of a photon and phonon, respectively. In what is commonly known as the rotating-wave approximation, the two (nonsecular) terms $a^\dagger b^\dagger + ab$ are often disregarded. Part of the justification for this process is that these terms, when considered individually, appear to be "non-energy-conserving". Though this is often an acceptable approximation, depending on the system setup, it may lead to qualitatively incorrect predictions. For example, in the absence of external driving and at low temperature, the term $a^\dagger b^\dagger$ may be a significant source of excited states, though understanding the nature of these states and when they may be useful requires a more careful analysis.

We investigate the contribution of such nonsecular terms to polariton physics and chemistry in both the coupling between the molecules and the cavity-supported mode (e.g., Rabi/Dicke vs. Jaynes–Cummings/Tavis–Cummings models) as well as in the coupling between the polariton system and its thermal environment (e.g., Lindblad vs. Redfield equations).

P137

A review of electrocatalysts for glycerol electrooxidation reactions: current advances and future perspectives

K branur Ağtoprak[1] , Ramiz Gültekin Akay[1]

[1]*Kocaeli University, Department of Chemical Engineering, Kocaeli, Türkiye*

Growing global interest in clean energy sources, aimed at reducing CO_2 emissions compared to traditional fossil fuels, has underscored the importance of fuel cell applications for a sustainable future. Consequently, R&D studies in fuel cell technology have been increased over the last 20 years.

Researchers worldwide have revealed that glycerol can be an effective fuel in alcohol fuel cells. The increase in demand for biodiesel production increases the production of its by-product, glycerol; typically resulting in 1 kg of glycerol for every 10 kg of biodiesel produced. Glycerol is a preferred fuel among various liquid fuel cells due to its high reactivity, energy density, and low toxicity. Catalyzed glycerol oxidation provides the formation of valuable by-products. Glycerol has the potential to provide renewable and ultra-clean energy through waste-to-wealth conversion. However, catalyst selection in the fuel cell anode chamber for best performance and high efficiency requires further research. Heretofore, catalysts containing Pt and Pd have been used in direct glycerol fuel cells (DGFC) as they provide high activity. However, alloying these noble metals with transition metals such as Sn, Co, Fe, Au, Ag, and Mn has offered many advantages.[1] Overall, this study examines the development of glycerol oxidation reaction electrocatalysts and DGFC. In addition, will shed light on their current advantages and future perspectives.

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P138

Syntheses and characterization of Cu(II) and Ni(II) coordination polymers constructed from flexible pamoic acid and ethylenediamine mixed ligands

Yasemin Tümer[1], Ahmed Kareem Khalaf[1], Ayşin Zülfikaroğlu[2], Çiğdem Yüksektepe Ataol[3]

[1]Karabük University, Department of Chemistry, Karabük, Turkey
[2]Amasya University, Department of Chemistry, Amasya, Turkey
[3] Çankırı Karatekin University, Department of Physics, Çankırı, Turkey

The design and construction of novel functional coordination polymers (CPs) or metal-organic frameworks (MOFs), have attracted a great deal of attention in recent decades due to their intriguing structures and elegant topologies. Ligands possessing distinct symmetry and varying degrees of rigidity/flexibility play a pivotal role in regulating and modifying the topologies of MOFs or CPs. Pamoic acid (H2pam) is a flexible dicarboxylic acid consisting of two naphthalene moieties connected by a methylene bridge. To reduce steric hindrance, the two naphthalene arms can freely rotate around the methylene (–CH2–) groups in accordance with slight changes in the coordination environment.[1,2] We selected ethylenediamine (en), which is a small, straight-chain and flexible ligand as auxiliary ligand.

We have synthesized two coordination polymers (1 and 2) by the reaction of pamoic acid, ethylenediamine, and transition metal salts (Ni and Cu) (Figure 1). The molecular and solid-state structures of 1 and 2 were established using single-crystal X-ray diffraction methods.

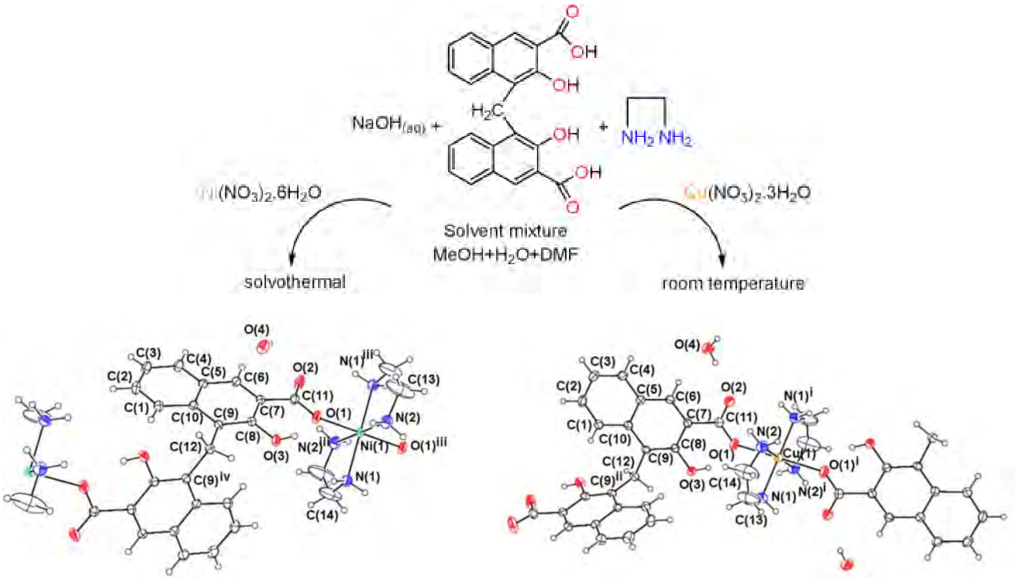

Figure 1: Syntheses of Cu(II) and Ni(II) coordination polymers (1 and 2) and ORTEP drawing including polymer coordinations of the moleculer structures

The author acknowledges the Karabük University Scientific Research Project Unit (Grant No. KBUBAP-23-YL-117).

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Cobalt complexes as structure-directing agent in the synthesis for zeolites

Janina Carolin Höner [1], Andreas Schaate [1], Yaşar Krysiak [1]

[1] *Leibniz University Hannover, Institute of Inorganic Chemistry, Hannover, Germany*

Zeolites have a wide range of applications i.e. as molecular sieve or catalysts for organic reactions. In order to design the properties of these materials, the pore size and form plays a decisive role. Structure-directing agents (SDAs), traditionally organic amines or alkylammonium salts, are used to control the zeolite formation. An emerging alternative, metal complexes, offers the potential to incorporate metal atoms into the silica framework during the removal of the SDA by the calcination process. These metal atoms can then serve as catalytically active centers in organic reactions.[1,2]

Deploying metal complexes comes with a lot of challenges. The stability of these complexes during the hydrothermal process is highly dependent on the pH value. In alkaline conditions, typically used for zeolite synthesis, higher temperatures tend to reduce the stability of the metal complex, resulting in an amorphous silicon product. In contrast, lower pH value or temperature may favor the formation of a crystalline product but the conditions for this are quite narrow.

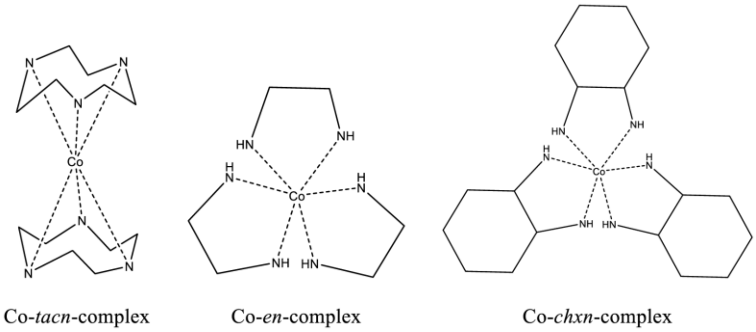

Figure 1: Schematic presentation of used cobalt(III)-complexes.

Octahedral cobalt complexes (Figure 1) were deployed as SDAs in various zeolite synthesis routes. The complexes can be used as SDA or as co-SDA in conjunction with traditional SDAs, like tetramethyl amine hydroxide, for known zeolite structure, such as zeolite A (LTA). Another way is to encapsulate the complex in the pore system of a zeolite framework. Further recrystallization then yields another zeolite structure. A notable result is the creation of LMU-2 (Ludwig-Maximilian University – 2) by using the $[Co(\mathit{tacn})2]^{3+}$ complex as structure directing agent and only silica as precursor in a typical hydrothermal synthesis yielding a yellow powder.[3] This zeolite, while similar to chabazite (CHA), exhibits an interrupted porous framework (–CHA) due to the large complex molecule located in its cages. The crystal structure of LMU-2 is determined by 3D electron diffraction and the hydrogen atom of the $[Si–O\cdots H\cdots O–Si]^-$ hydrogen bond of the interrupted framework, whose position could previously only be calculated by molecular modelling, can be located by using this method.

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P140

Isolation of an *n*-Alkane Complex from Solution: Competition with the Weakly Coordinating Solvent

Malte Sellin [1], Julia Fischer [1], Ingo Krossing [1]

[1] *University of Freiburg, Institute of Inorganic and Analytical Chemistry, Freiburg, Germany*

Alkanes are poor ligands for transition metals, with the only possible electron-donation from the C–H σ bonds, which are assigned to energetically low-lying orbitals. On the other hand, the LUMOs of alkanes are too high to receive electron density from the HOMO of the metal centre.[1] Therefore, the coordination power of alkanes is exceeded by the most counterions and solvents. Consequently, alkane complexes have been hitherto only observed in low temperatures matrices[1], with short lifetimes[2] in solution or in single-crystal to single-crystal[3] reactions.

To nevertheless isolate an alkane-complex from solution, both the solvent and counterion must have a low basicity. To meet this requirement, we used a combination of a very large and weak polarisable perfluoroalkoxyaluminate based anion $[Al(OR^F)_4]^-$ ($R^F = -C(CF_3)_3$) and polar but weakly coordinating fluorinated benzene derivative 1,2,3,4-Tetrafluorobenzene (4FB). To afford a highly Lewis-acidic 16-VE-fragment, $Mn_2(CO)_{10}$ was deelectronated using Ag^+, yielding the desired complex $[Mn(CO)_5(n\text{-pentane})]^+$.

Still, also the solvent complex $[Mn(CO)_5(4FB)]^+$ is formed as a minor-product, underlining the strong competition between the solvent and the alkane. While DFT-calculations are showing a preference of the $[Mn(CO)_5]^+$ towards 4FB in the gas-phase, considering solvation effects on the other hand are supporting the experimental findings of the $[Mn(CO)_5(n\text{-pentane})]^+$ complex as main-product.

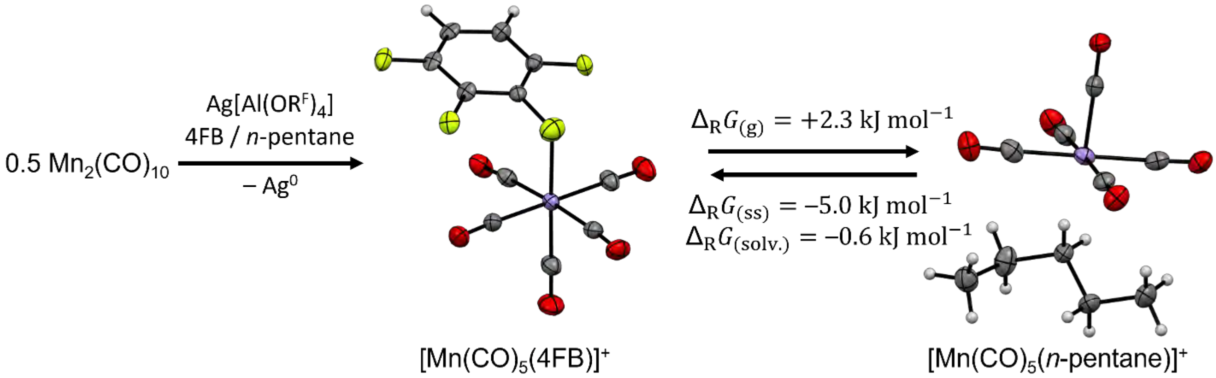

Figure 1: Deelectronation of $Mn_2(CO)_{10}$ and the resulting equilibrium between $[Mn(CO)_5(n\text{-pentane})]^+$ and $[Mn(CO)_5(4FB)]^+$.

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P141

Differences in Emulsion Polymerization Fouling between Acrylates and Vinyl Acetates Studied In-Situ with a Quartz Crystal Microbalance (QCM)

Kevin M. Hoffmann[1], Arne Langhoff[1], Jörg Adams[1], Holly A. Huellemeyer[2], Wolfgang Augustin[2], Diethelm Johannsmann[1]

[1] Clausthal University of Technology, Institute of Physical Chemistry, Clausthal-Zellerfeld, Germany

[2] Technical University of Braunschweig, Institute for Chemical and Thermal Process Engineering, Braunschweig, Germany

Using a quartz crystal microbalance with dissipation monitoring (QCM-D), fouling during emulsion polymerization was followed *in-situ*. The quartz resonator was heated from the back with a ring-shaped thermal pad, which turns the resonator into a heat-transfer surface.[1] We compare the emulsion polymerization of acrylates, stabilized with the non-ionic surfactant Lutensol AT50 and vinyl acetates, stabilized with the protective colloid polyvinyl alcohol.

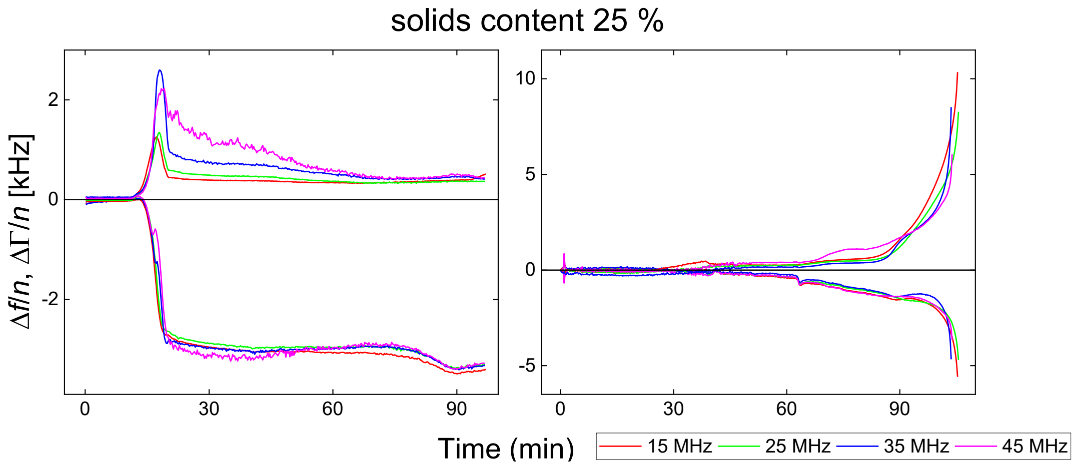
solids content 25 %

Figure 1: Frequency and bandwidth shift during emulsion polymerization of acrylates (BA-MMA, left) and vinyl acetate (right).

For the acrylates, we mostly find self-limiting fouling layers, meaning that the layer remains finite in thickness. The thickness is in the range of the particle diameter. This type of fouling is unproblematic for the practical process. For vinyl acetate, the fouling layer keeps growing, as also evidenced *ex-situ* in form of a material almost filling the reaction vessel. At this point, we assume self-limiting layers when particle fouling is present (according to LANGMUIR). When reaction fouling is present, we expect fouling layers which diverge in thickness. The mechanism leading to stable layers of finite thickness is under investigation.

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