Innovation in chemical sciences : book of abstracts

INNOVATION IN CHEMICAL SCIENCES

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Book of Abstracts

Foreword

The primary aim of the Symposium *Innovation in Chemical Sciences* was to create a collaborative platform for researchers and students from the University of Zagreb and the University of Regensburg, enabling them to share the latest findings, developments, and achievements in the field of chemistry. The vision was to establish a more informal setting that included Master's, PhD, and Postdoctoral students to encourage cooperation and foster mobility.

As the symposium evolved, it welcomed not only participants from the University of Regensburg but also researchers from other Bavarian universities and the University of Toulouse. In the end, the symposium featured a total of 20 oral presentations and 20 poster sessions, offering a diverse and enriching exchange of ideas.

This book compiles the abstracts of the talks and posters presented at the *Innovation in Chemical Sciences* symposium, held in Zagreb, Croatia, from November 19–21, 2024.

Nikola Cindro, Nikolas Djukic, Burkhard König & Jana Pisk

Acknowledgements

We are grateful to all those who supported the symposium *Innovation in Chemical Sciences*. Your contributions have been invaluable, and we sincerely appreciate your commitment to making this event a success.

Sveučilište u Zagrebu

Universität Regensburg

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Programme and Scientific Committee

Associate Professor **Dominique Agustin**, University of Toulouse, IUT P. Sabatier, Toulouse III

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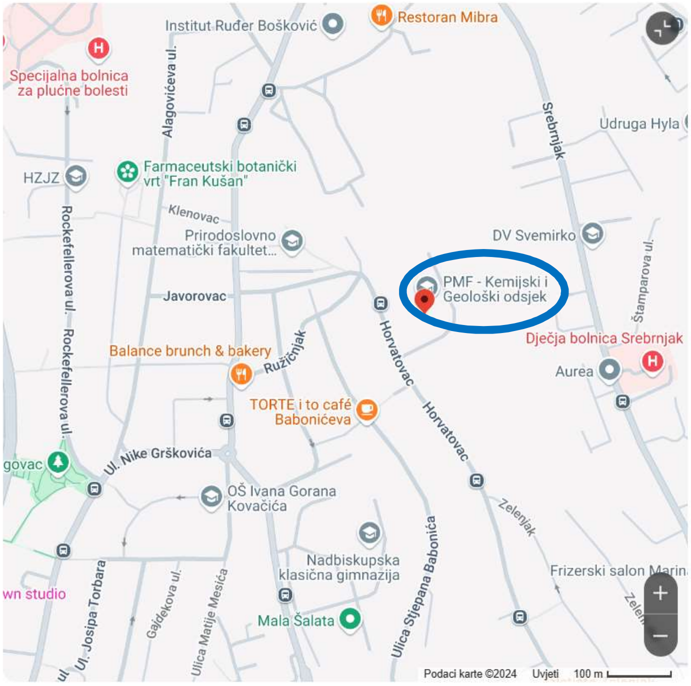
Associate Professor **Jana Pisk**, University of Zagreb, Faculty of Science, Department of Chemistry

Professor **Oliver Reiser**, University of Regensburg, Faculty of Chemistry and Pharmacy

Symposium venue

The symposium will be held University of Zagreb, Faculty of Science, Department of Chemistry, Horvatovac 102a, 10000 Zagreb.



Program

DAY 01 (19.11.2024) TUESDAY **Hall P1**	
13:00 – 14:00 Gathering at the PMF (Horvatovac 102a) and refreshment	
14:00 – 14:30	Opening remarks
14:30 – 14:55	Oliver Reiser: *Turning Hay to Gold: Catalytic conversion of non-edible renewable resources into value-added product*
14:55 –15:20	Dominik Cinčić: *Crystal engineering of organic and metal-organic halogen-bonded cocrystals*
15:20 –15:55	Burkhard König: *Better organic synthesis with light*
15:55 – 16:10 Coffee break	
16:10 – 16:35	Aleksandra Maršavelski: *Ancestral Sequence Reconstruction as a Tool to Enhance Solubility and Yield of Polyester-Degrading Enzymes*
16:35 – 17:00	Patrick Nürnberger: *A Time-Resolved Look on Photochemical Processes for which Adjacent Molecules Play a Crucial Role*
17:00 – 17:15	Ali Haidar: *Green Catalysis for Biomass-Derived Heterocycles: Solvent-Free Oxidation of Linalool Using Polyoxometalates*
17:15 – 17:30	Nils Dünninger: *Synthesis of GaPt alloys supported on spray-dried supraparticles assembled to hierarchical suprabeads*
17:30 – 17:45	Gregor Talajić: *Total synthesis of Penicyclone A*
17:45 – 18:30 Aperitive	
19:30 Dinner	
Day 02 (20.11.2024) WEDNESDAY **Hall P1**	
9:00 – 9:25	Julia Rehbein: *Alice's Adventures in PhysOrg-Land*
9:25 – 9:50	Dominique Agustin: *Solvent-Sober Catalytic Processes for Biomass Valorization*
9:50 – 10:15	Michael Bodensteiner: *Anomalous crystallography - can we see oxidation states in crystal structures?*
10:15 – 10:30	Florian Meurer: *Quantum Crystallography as a Chemist's Tool for Bond Analysis*
10:30- 10:45 Coffee break	
10:45 – 11:10	Gábor Balázs: *The Manifold Reactivity of Polyphosphorus Complexes*
11:10 – 11:35	Ivana Biljan: *Thin films and porous organic polymers built from aromatic compounds with nitrogen functionalities*
11:35 – 12:00	Dominik Horinek: *Molecular dynamics of solvent effects on ions, ion pairs, and ion aggregates*

12:00 – 12:15	Andrea Usenik: *The challenges behind solutions: An insight from various viewpoints of supramolecular physical chemists*
12:15 – 13:15 Lunch break	
13:15 – 13:40	Frank-Michael Matysik: *(Bio)Analytical Chemistry and Sensor Research at Regensburg University: An Overview*
13:40 – 14:05	Svetlana B. Tsogoeva: *Achieving molecular complexity via metal-free domino reactions*
14:05 – 14:30	Stefan Kalkhof: *Guiding Biomaterial Design through the Power of Omics Technologies*
14:30 – 14:45	Evgeniia Dorinova: *Site-specific RNA modifications by catalytic RNAs*
14:45 – 15:00	David Klarić: *Application of mass spectrometry in characterization of drug: β-cyclodextrin systems*
15:15 – 15:30 Coffee break	
15:30 – 17:30	Flash poster and poster session (entrance lobby)
17:30 – 19:00 Sightseeing of Zagreb	
19:00 Dinner	
Day 03 (21.11.2024) THURSDAY **Room 222**	
9:00 – 10:00	Poster session (entrance lobby)
10:00 – 11:30	Round table about future collaboration and cooperation/closing remarks
11:30 Refreshment	

List of participants

Agustin Dominique
Bagheri Ali
Balázs Gábor
Biljan Ivana
Bodensteiner Michael
Brtan Lucija
Cinčić Dominik
Cindro Nikola
Đilović Ivica
Djukic Nikolas
Dorinova Evgeniia
Dulić Morana
Dünninger Nils
Duvnjak Mirko
Eshagi Iman
Frey Tea
Galić Nives
Gregor Talajić
Haidar Ali
Horinek Dominik
Huf Elisabeth
Ilić Nikolina
Juračić Tea
Kalkhof Stefan
Klarić David
Koenig Burkhard
Korade Karla
Kožić Matej
Kukina Gradečak Karla
Liović Marin
Mandarić Mirna
Markoč Paula
Maršavelski Aleksandra
Matysik Frank-Michael
Meurer Florian
Močibob Marko
Nikolić Juraj
Nuić Laura
Nürnberger Patrick
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Pisk Jana

Pocrnić Marijana
Popović Matija
Pulido-Díaz Israel T.
Rehbein Julia
Reiser Oliver
Rosenhammer Martin
Sarjanović Josipa
Schedlowski Sven
Schiller Julian
Škalamera Đani
Soliman Basant
Sovulj Gruić Ita
Toplak Juraj
Tsogoeva Svetlana B.
Usenik Andrea
Zwolenik Aleksandra

Agustin Dominique Oral presentation

Solvent-Sober Catalytic Processes for Biomass Valorization

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The current critical situation on climate (greenhouse gases, global warming, etc.) [1] due to non-reasonable resource use (fossil ones, metals, etc.) on our planet encourages the EU to propose sustainable processes to avoid an unsustainable future.[2] For reasonable chemical production, processes that are sober in energy/metals/fossil materials are one thematic presented here.[3] Thus, the study of the catalytic activity of compounds containing molybdenum[4,5] and/or vanadium[6,7] for the oxidation of model compounds - in mild conditions and without organic solvent – led to mechanisms understanding[4,7] and catalyst improvements.[8] The work was extended to biomass valorisation[9] and grafting of complexes on supports for recycling.[10]

Literature

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Biography

After defending PhD in Toulouse, Dominique did a post-doctoral stay in Saarbrücken (group of M. Veith) then started his permanent academic career as assistant professor in Paris (Univ. Pierre et Marie Curie) before joining Castres (Univ. Paul Sabatier) where he became associate professor after defending his habilitation. Within one LCC-CNRS research group, his research includes catalysis, green chemistry, biomass valorization, catalyst grafting and DFT calculations. He is involved in several bilateral projects including two projects with Croatia, SOSOPRO and SusPolMoV. He is Vice-President of the Sustainable Chemistry Division of French Chemical Society.

The Manifold Reactivity of Polyphosphorus Complexes

Gábor Balázs[1]

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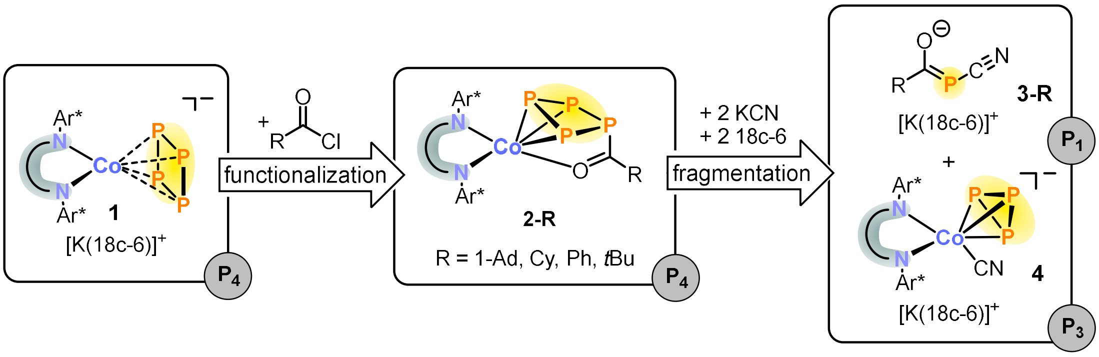
White phosphorus (P_4) is the most reactive allotrope among the room-temperature-stable modifications of element 15 and an important commodity chemical.[1] The annual production of P_4 exceeds 1 Mt, and this pivotal industrial role inspires the development of new transformations.[2] The group Prof. Robert Wolf at Regensburg University develops new catalytic P_4 functionalization procedures to generate valuable monophosphorus products. In addition, we also seek to access previously unknown organophosphorus compounds by functionalizing P_4 in the coordination sphere of transition metals.

This talk will give an overview of the research activities in the Wolf group. Among other work, we will describe the functionalization of P_4 ligands in the coordination sphere of cobalt (Scheme 1).[1,2] Inspired by the relevance of acyl-substituted monophosphorus compounds as photoinitiators, we have developed transition metal-mediated procedures for the preparation of previously unaccessible acylcyanophosphines.[3,4]



Scheme 1. Acylation and subsequent [3+1] fragmentation of white phosphorus.

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Biography

Gábor Balázs was born in Branistea, Romania. After undergraduate studies at the Babes-Bolyai University (Cluj-Napoca, Romania), he received his Ph.D. under the supervision of Prof. H. J. Breunig at the University of Bremen (Germany) in 2002. From March 2003 to October 2005, he was a postdoctoral associate of Prof. M. Scheer in Karlsruhe and then Regensburg (Germany). In October 2005, he joined Professors D. M. P. Mingos and J. C. Green at Oxford University as a postdoctoral research fellow supported by the Alexander von Humboldt foundation. This was followed by a postdoctoral stay in the group of Prof. M. Driess in Berlin (Germany). In 2008, he returned to Regensburg to join Prof. M. Scheer’s group as a senior researcher. Since 2022, he has been associated with the group of Prof. R. Wolf in Regensburg.

Thin Films and Porous Organic Polymers Built From Aromatic Compounds With Nitrogen Functionalities

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The construction of functional materials with the desired properties using a bottom-up approach is based on connecting the smaller building units of predetermined geometry and functionality in a predictable manner. In our research, we use structurally similar building units, aromatic compounds with nitrogen functionalities, for the design of thin films with possible application in the fabrication of electronic devices and porous organic polymers for CO_2 adsorption.

Due to their ability to dimerize and polymerize via azodioxy bonds, aromatic C-nitroso compounds can be used for the preparation of bilayer and multilayer films on surfaces. In the first part of the lecture, an overview of recent studies on self-assembly, dimerization and polymerization of aromatic C-nitroso compounds on gold surfaces and the formation of nitroso/azodioxy films will be given. [1–3]

Increased emissions of carbon dioxide (CO_2) into the atmosphere are considered a major environmental challenge due to their contribution to global warming and climate change. Porous organic polymers containing nitrogen-rich functionalities have recently emerged as promising candidates for CO_2 capture and sequestration. The second part of the lecture will focus on the synthesis and characterization of new porous organic polymers with nitrogen-nitrogen linkages which could be used as CO_2 adsorbents. [4–6]

This work has been fully supported by Croatian Science Foundation under the project IP-2020-02-4467.

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Biography

Ivana Biljan received her PhD degree from the University of Zagreb, Faculty of Science in 2009. During 2010 and 2011 she spent 17 months as a postdoctoral researcher at the National Institute of Chemistry in Ljubljana, Slovenia.

Since 2003, she has been employed at the Department of Chemistry, Faculty of Science. University of Zagreb. In 2020, she was promoted to Associate Professor.

Her research deals with the synthesis and characterization of new aromatic C-nitroso derivatives and porous organic polymers with nitrogen-nitrogen linkages, self-assembly of molecules on surfaces and preparation of thin films, atomic force microscopy, scanning tunneling microscopy and NMR spectroscopy.

She has published more than 30 peer-reviewed journal articles and co-authored more than 80 poster and oral presentations. She has given 1 plenary and 9 invited talks at scientific conferences. She was involved as a research associate in numerous scientific projects, and she is a principal investigator of 1 ongoing research project.

Ivana Biljan participates in organic chemistry classes. She supervised 4 PhD theses (2 completed and 2 in progress), 15 diploma theses and 10 bachelor theses.

Anomalous crystallography - can we see oxidation states in crystal structures?

Michael Bodensteiner[1]

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Crystal structure analysis is probably the most important method for structure elucidation in many areas of chemistry and beyond. Compared to other analytical methods, X-ray structure analysis requires a structure model to be created on the computer and optimized against the measured data. Approximations and corrections are used both for the measurement data and for the structural models. Until now, almost exclusively spherical electron density distributions have been used to describe the atoms in the model. Charges, bonds and free electron pairs are completely ignored. However, it is perfectly possible to incorporate all these features into the model and significantly improve the quality of the resulting structures, even with normal data that can be obtained on virtually any diffractometer.[1] An absorption correction is carried out for all structure determinations, which takes into account the fact that not all photons are diffracted but are instead absorbed. This absorption correction is in turn directly related to the correction for anomalous dispersion effects, but this is applied to the model and not to the data. Therefore, both effects contribute to the apparent discrepancy between the number of electrons diffracted and the actual number present.[2] Conversely, this effect can also be employed to determine whether an atom has a lower electron count than expected indicative of a higher oxidation state.

Literature

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Bodensteiner Michael Oral presentation

Biography

Michael Bodensteiner is Head of X-ray Structure Analysis at the Central Analytical Laboratory of the University of Regensburg. He studied chemistry at the University of Regensburg, where he obtained his PhD in inorganic chemistry in 2011. Since then, he has been responsible for crystallography at the Faculty of Chemistry and Pharmacy. Since April 2022, he has been a habilitation candidate in inorganic chemistry and his research focuses on improving crystal structure determination and gaining more information from it. He is particularly interested in quantum crystallography, anomalous dispersion and absorption effects, and the crystalline sponge method. He is also the managing director of the German branch of the company OlexSys, which develops the most widely used structure refinement programme for small molecules, Olex2.

Ancestral variants of the MGY enzyme showed significantly improved solubility and expression yields

Lucija Brtan,[1] Margaux Aubel[2], Erich Bornberg-Bauer[2], Ivana Kekez[1], Aleksandra Maršavelski[1]

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Over the years, plastic pollution has become an increasing problem for both the environment and human health.[1] The urgent need for sustainable solutions to plastic pollution has led to a surge in research on enzyme-driven biodegradation of synthetic polymers, particularly polylactic acid (PLA).[2] In this study, we identified a novel enzyme, MGY, from a metagenomic database for its PLA-degrading ability. However, limited solubility and low yield of the MGY enzyme hindered further structural and functional analysis. To improve its solubility and yield, we applied ancestral sequence reconstruction, generating three ancestral MGY variants – 118_CLU, 119_CLU, and 121_CLU. These ancestral variants retained high PLA-degrading activity, as verified through activity assays on emulsified PLA plates, making them more suitable for practical applications and detailed structural studies. Transformation of electrocompetent bacteria with the vector containing synthetic genes of the specific enzymes, followed by cultivation and protein expression, demonstrated that sequence modification by ancestral reconstruction increases protein solubility, and contribute to the higher expression yield. The enhanced solubility and expression of these ancestral MGY variants highlights ancestral sequence reconstruction as a powerful tool, providing a pathway for developing effective biocatalysts for PLA recycling and environmental sustainability, facilitating both applied and structural studies.

Literature

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Biography

Lucija Brtan is a PhD student and Expert Associate at the Biochemistry Division, Department of Chemistry, Faculty of Science, University of Zagreb (Croatia), specializing in protein engineering, with expertise in protein purification and crystallization techniques. Currently, Lucija is contributing to the project Enzyme Engineering for Sustainable Bioplastic Recycling (NPOO.C3.2.R2-I1.06), which aims to develop enzyme-based solutions for bioplastic recycling. Her research focuses on identifying and characterizing metagenomic (poly)esterases with potential activity against polylactic acid (PLA), the most widely used bioplastic polymer.

Crystal Engineering of Organic and Metal-Organic Halogen-Bonded Cocrystals

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Over the past three decades, research into halogen bonding has been intensified in all fields of chemistry, especially in supramolecular chemistry and crystal engineering.[1] Solid-state studies have been fundamental for the understanding of halogen bonding, with crystallography as the most important tool. Particularly, cocrystallization has offered insight into the influence of varying donors and acceptors on the halogen bond properties. Studies on halogen-bonded cocrystals have mostly focused on organic systems with perfluorinated compounds as halogen bond donors, and a variety of organic acceptors involving nitrogen atoms and oxygen.[2] The use of halogen bonding to direct the assembly of metal complexes (coordination compounds) as acceptors or donors in cocrystals remains largely unexplored.[3] From the crystal engineering point of view, metal complexes represent extremely intriguing building blocks, they provide a plethora of geometries not normally accessible to organic molecules thus providing a wider range of accessible supramolecular architectures. Our group is focusing on developing halogen bonding as a tool in crystal engineering of multi-component solids through the involvement of new acceptor and donor types, notably the incorporation of metals into halogen-bonded structures. Designing cocrystals with neutral metal complexes as components presents a considerable challenge by both crystallization from solution and mechanochemical methods. This presentation will provide an overview of some of the work related to metal-based halogen-bonded cocrystals that we have pursued recently – evaluation and comparison of halogen bond proclivity of halogenide and pseudohalogenide ligands in metal complexes[4,5] and the potential of metal chelates as halogen bond acceptors or donors in crystal engineering of metal-organic multicomponent solids.

Literature

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Biography

Dominik Cinčić is a Full Professor at the University of Zagreb, Faculty of Science, Department of Chemistry. He received his Ph.D. (2009) at the University of Zagreb with Professor Branko Kaitner. In 2007, he was a visiting researcher at the University of Cambridge under the supervision of Professor William Jones and Professor Tomislav Friščić. He is experienced in crystallization of molecular solids, cocrystal and salt screening of pharmaceuticals, mechanochemical and solvent-free synthesis of diverse organic and metal-organic materials. Current research in his group is focused on crystal engineering of multicomponent halogen-bonded organic and metal-organic materials. He has authored over 80 scientific publications and over 200 oral and poster presentations at national and international conferences. He has also been active in science popularization since 2007, participating in the annual "The Magic in Chemistry" and "Open day of the Chemistry Department" events. He was the recipient of the Croatian National Science Award for outstanding scientific discoveries in the field of supramolecular chemistry – halogen-bonded solids (2018) and the annual award ‘Brdo‘ for the best teacher at the Department of Chemistry, administered by the Student Association at the Faculty of Science (2013, 2014, 2016, 2017, 2020, 2021 and 2023).

Mechanochemical Synthesis of A-Acylamino Benzamide

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In recent years, there has been increasing recognition of microwave-assisted and mechanochemical synthesis due to their eco-friendly nature and alignment with the principles of green chemistry.[1] In the Ugi multicomponent reaction[2] different amines, aldehydes or ketones, carboxylic acids and isocyanides combine to α-acylamino amides.

In this work, mechanochemical synthesis of the *N*-benzyl-*N*-[(*tert*-butylaminocarbonyl)methyl]benzamide (**1**) and *N*-isobutyl-*N*-[(cyclohexyl aminocarbonyl)methyl]benzamide (**2**) was performed through the Ugi reaction. Mechanochemical synthesis of compounds **1** and **2** was performed using a ball mill without solvents and/or with a catalytic amount of solvent (known as liquid-assisted grinding, LAG).[1] The obtained products were characterized by standard analytical methods (FTIR, 1D, 2D NMR, HRMS). The purity of the obtained products was checked by HPLC method. The inhibitory activity (IC_{50} values) of all prepared compounds toward the butyrylcholinesterase isolated from horse serum was measured by Ellman method.[3]

Literature

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Biography

Toni Divjak graduated in 2023. from the Department of Chemistry, Faculty of Science, the University of Zagreb with a diploma thesis *Design and preparation of imidazole, pyrazole and 5-methylisatin acetylcholinesterase reactivators* under the mentorship of Dr. Dijana Pešić. He enrolled in doctoral studies in chemistry (field of Organic Chemistry) in 2023.

He has been working as a research and teaching assistant at the Division of Organic Chemistry since 2023. He was the assistant mentor of two diploma theses and one final exam. His scientific research involves the synthesis and characterization of peptidomimetics by Ugi reaction.

Site-specific RNA modifications by catalytic RNAs

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Post-transcriptional RNA modifications are crucial regulatory elements which define RNA folding, functions and influence gene expression. Among them, methylation is one of the utmost important RNA epitranscriptome modifications found in all types of RNA (mRNA, rRNA, tRNA), often at evolutionary conserved positions. In nature, protein enzymes use nucleotide-derived cofactors such as S-adenosylmethionine (SAM) as a universal methyl group donor to catalyse a methylation reaction. In the context of origin of life, RNA was predominantly considered as the main biopolymer responsible for both functions: storage of genetic information and catalysis. Such catalytic RNA molecules known as RNA enzymes or ribozymes are found in nature where they mostly perform phosphodiester transfer reactions, whereas artificially made ribozymes provide potential for more diverse functions. In addition to natural protein enzymes, methyltransferase activity can be reconstituted in the laboratory by in vitro selection from a random RNA library. In this regard, a breakthrough has been achieved when the first ribozyme mimicking protein methyltransferase activity has been identified in the Höbartner group.[1] This methyltransferase ribozyme (MTR1) site specifically methylates an external RNA at N1 position of a specific adenosine to generate 1 methyl-adenosine (m1A) utilizing O6-methylguanosine as a small molecule cofactor.[1] Subsequently, the crystal structure of the ribozyme was solved in a post-catalytic state and revealed an intriguing catalytic mechanism involving a protonated cytidine.[2] MTR1 accepts various target sequences as RNA substrates including native tRNAs thus producing natural m1A modification in tRNA. In order to expand the scope of RNA alkylation and install other different RNA modifications by catalytic RNAs, new in vitro evolution was performed. The new in vitro selection experiments were aimed to evolve novel ribozymes catalysing an attachment of an alkyl group at a different target site in the substrate RNA beyond m1A produced by MTR1. In this work, we identified and extensively characterised a new RNA-modifying ribozyme which enables efficient site-specific RNA alkylation and serves as an additional RNA-labeling protein free tool in vitro.

Literature

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Biography

Evgeniia Dorinova studied Organic Chemistry at the Lomonosov Institute of Fine Chemical Technologies, Moscow. During her bachelor's and master's studies, she worked at the Engelhard Institute of Molecular Biology, RAS, Moscow where she was involved in the development of an environmentally friendly method for synthesis of biologically important nucleosides based on enzymatic transglycosylation. She received the Master's Degree in Organic and Medicinal Chemistry in 2020 and decided to join the Höbartner group in Würzburg to pursue her Ph.D studies. In 2021, Evgeniia was awarded a BAYHOST Fellowship which financially supports her as a Ph.D student at the University of Würzburg, Germany. Her current research project focuses on in vitro selection of novel modified ribozymes for site-specific RNA-alkylation and labeling.

Mechanochemical Chloride-Assisted Peptide Macrocyclization

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Cyclic peptides have garnered significant attention in recent years due to their enhanced biological activity compared to linear peptides. The rigidity of the cyclic structure increases their *in vivo* stability and bioavailability, making them promising candidates in drug development.[1] One of the main methods of obtaining cyclic peptides is head-to-tail lactamization of linear precursors which requires the use of templating agents to induce conformational reorganization, bringing the reactive *N*- and *C*-termini in close spatial proximity, thus facilitating the macrocyclization step.[2] Our previous research has shown that anions have the ability to bind to linear and cyclic oligopeptides (in addition to the well-known binding ability of cations) which was utilized for the preparation of several cyclic tetra-, penta- and hexapeptides.[3]

In this work, we prepared three oligopeptides by conventional solution-based methods: Phe-Phe-Gly-Gly (**1**), Phe-Phe-Gly-Gly-Phe (**2**) and Phe-Phe-Gly-Gly-Phe-Phe (**3**) and the corresponding cyclopeptides **C2** and **C3** were obtained, while **1** failed to cyclize. A mechanochemical approach was developed in which the linear peptide is milled with a quaternary ammonium salt, followed by addition of the coupling reagent DEPBT, yielding the corresponding cyclic peptide in significantly reduced reaction times – from days to hours. Additionally, this approach circumvents high-dilution conditions and the poor solubility of linear precursors in typical organic solvents; problems which the solution-based methods suffer from. To better understand the role of the chloride salt in this process, we conducted IR spectroscopy experiments and molecular dynamics simulations of the peptide-chloride complexes.

Literature

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Duvnjak Mirko Poster presentation

Biography

Mirko Duvnjak, born on August 7, 1999, in Zagreb, Croatia, is a dedicated researcher in the field of chemistry. He is currently working as a research associate on a scientific project at the Faculty of Science, University of Zagreb, in the Department of Organic Chemistry. Duvnjak completed his Master's degree in Chemistry, specializing in inorganic and organic chemistry, in 2023, following his undergraduate studies at the same institution.

Throughout his academic journey, Duvnjak has received several prestigious awards, including the Dean's Award and the Chemistry Department Medal in 2023 for academic excellence. In 2022, he was honored with the Rector's Award for his research on oligopeptide synthesis and macrocyclization. He has also been recognized for his achievements in national chemistry competitions and the European Union Science Olympiad. Duvnjak has actively participated in scientific conferences and presented his research on cyclopeptides and their binding properties, contributing to advancements in supramolecular chemistry.

SUIPLiER - Sustainably Usable Inter-Processual Lignin Erlangen

Contribution to sustainable pulp use – extraction of lignin from black liquor

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The submission to the VDI (Association of German Engineers) chemPLANT student competition from 2023 presents a concept for the material recycling of black liquor in the paper industry. The process developed, called SUIPLiER (Sustainably Usable Inter-Processual Lignin Erlangen), aims to obtain an easily separable intermediate product, kraft lignin, from the black liquor. Once extracted from the Kraft process, this bio-based polymer is considered an important raw material for the renewable production of polymers, adhesives, coatings and other products. It also offers numerous other potential applications, such as the replacement of asphalt or further processing into carbon fibers.

In the SUIPLiER process, separation takes place in two streams. In the first stream, the lignin is concentrated and separated as a valuable product, while in the second stream the remaining organic components are removed, and the inorganic components remain dissolved in the water. The aim is to minimize water consumption and avoid unnecessary energy flows.

The process begins with the addition of black liquor as a feed, which is cooled and then nanofiltered. By using this membrane separation technology, energy-intensive evaporation and rectification processes can be avoided. The retentate contains the concentrated lignin, which is precipitated by lowering the pH value in the Venturi gas scrubber. The solid and liquid components are separated, and the solid lignin is washed and concentrated. The solid lignin is recovered by evaporation.

The permeate from the nanofiltration is treated in a similar way and the liquid from the separators is fed together into an absorber column with CO_2 in counterflow to further reduce the pH value. The resulting biogas is used to generate energy. The fermentation residue from the biogas plant is separated and the solids are thermally utilized. The liquid phase is heated to expel the CO_2 and obtain the green liquor. Neutralization takes place in the scrubber and in the absorption column. The white liquor is reused in paper production.

The SUIPLiER process is characterized by a high degree of flexibility, as the lignin yield can be adjusted through additional nanofiltration stages depending on market demand and price developments. Another advantage of the process is the sustainable use of resources. The recycling of the lignin does reduce the amount of energy available in the plant. However, this is not an obstacle, as the utilization of the remaining organics provides enough energy for the operation of the plant and even exceeds it. Energy consumption can be further reduced through more efficient water management, which is in line with the goal of climate-neutral production. The SUIPLiER process offers not only ecological but also economic benefits. By recycling the lignin, a material previously regarded as waste is turned into a valuable product.

Overall, this work shows that the SUIPLiER process is a promising solution for the recycling of black liquor in the paper industry. Through the integration of product streams, the reduction of energy requirements and the sustainable use of resources, the process can offer both ecological and economic advantages. Further investigations and experimental verifications are necessary to ensure the practical suitability of the process and to identify further optimization potential. The SUIPLiER process offers a promising perspective for the paper industry to achieve its sustainability goals while remaining profitable.

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Dünninger Nils Poster presentation

Biography

My name is Nils Dünninger, currently a Master's student at the Friedrich-Alexander-Universität Erlangen-Nürnberg in the subject “Chemical Engineering - Sustainable Chemical Technologies”. Born on May 2nd, 2001 in Haßfurt (Bavaria, Germany), I started my studies in Chemical Engineering at the Friedrich-Alexander-Universität Erlangen-Nürnberg in October 2019 after graduating from high school. I completed my Bachelor's degree in August 2023, while I had already been enrolled in the consecutive Master's program since April 2023. My Bachelor's thesis was written at the Chairs of Chemical Reaction Engineering (Faculty of Engineering) and Inorganic Chemistry (Faculty of Natural Sciences) on the topic “Synthesis of GaPt alloys supported on spray-dried supraparticles assembled to hierarchical suprabeads”. The scientific paper “Supraparticles on beads for supported catalytically active liquid metal solutions - the SCALMS suprabead concept” was written by the supervisors of the thesis and will be presented in my talk.

For more than two years I have been working as a research assistant at the Chair of Chemical Reaction Engineering at the Friedrich-Alexander-University Erlangen-Nuremberg in the laboratory with SCALMS catalysts. Last year I spent three months as an intern in the “Technology & Innovation” department at Hydrogenious LOHC Technologies, a company that deals with the storage of hydrogen in organic liquids. At the end of 2023, I spent a semester abroad in Turku, Finland.

Synthesis of GaPt alloys supported on spray-dried supraparticles assembled to hierarchical suprabeads/

Supraparticles on beads for supported catalytically active liquid metal solutions – the SCALMS suprabead concept

Thomas Zimmermann,[1] Nnamdi Madubuko,[2] Philipp Groppe,[1]
Theodor Raczka,[1] Nils Dünninger,[1,2] Nicola Taccardi,[2] Simon Carl,[3]
Benjamin Apeleo Zubiri,[3] Erdmann Spiecker,[3] Peter Wasserscheid,[2,4,5]
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[5] Forschungszentrum Jülich, "Helmholtz-Institute Erlangen-Nürnberg for Renewable Energies" (IEK 11), Egerlandstr. 3, 91058 Erlangen, Germany

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Dünninger Nils Oral presentation

A novel GaPt-based supported catalytically active liquid metal solution (SCALMS) material is developed by exploiting the suprabead concept: Supraparticles, i.e. micrometer-sized particles composed of nanoparticles assembled by spray-drying, are bonded to millimeter-sized beads. The suprabeads combine macroscale size with catalytic properties of nanoscale GaPt particles entrapped in their silica framework.

In this work, it is proposed for the first time to lift the size of micrometer-scaled particles by supporting them on a millimeter-sized bead to create advanced catalyst-support entities, called suprabeads. This approach increases the size of the units while maintaining the unique properties of the micron-sized particles. While this idea is familiar for supported nanoparticles, attaching µm-particles to a support material requires completely dissimilar, novel synthetic procedures because of the different size regimes and thus, dissimilar physicochemical forces involved in binding the individual species. This concept extends the applicability of µm-scale particles in catalysis and many other fields. Here, it was implemented to synthesize a catalyst-support unit in which catalytically active µm-sized supraparticles are supported on mm-beads. The supraparticles, which represent a relatively recent and unique class of multifunctional materials, consist of assembled SiO2 and Ga (or GaPt) nanoparticles. Additionally, the possibility to spray-dry gallium dispersions to create supraparticles with enclosed gallium particles or droplets, depending on the temperature of the environment, was shown for the first time. This offers a new approach for generating catalytically active materials.

Literature

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Biography

My name is Nils Dünninger, currently a Master's student at the Friedrich-Alexander-Universität Erlangen-Nürnberg in the subject “Chemical Engineering - Sustainable Chemical Technologies”. Born on May 2nd, 2001 in Haßfurt (Bavaria, Germany), I started my studies in Chemical Engineering at the Friedrich-Alexander-Universität Erlangen-Nürnberg in October 2019 after graduating from high school. I completed my Bachelor's degree in August 2023, while I had already been enrolled in the consecutive Master's program since April 2023. My Bachelor's thesis was written at the Chairs of Chemical Reaction Engineering (Faculty of Engineering) and Inorganic Chemistry (Faculty of Natural Sciences) on the topic “Synthesis of GaPt alloys supported on spray-dried supraparticles assembled to hierarchical suprabeads”. The scientific paper “Supraparticles on beads for supported catalytically active liquid metal solutions - the SCALMS suprabead concept” was written by the supervisors of the thesis and will be presented in my talk.

For more than two years I have been working as a research assistant at the Chair of Chemical Reaction Engineering at the Friedrich-Alexander-University Erlangen-Nuremberg in the laboratory with SCALMS catalysts. Last year I spent three months as an intern in the “Technology & Innovation” department at Hydrogenious LOHC Technologies, a company that deals with the storage of hydrogen in organic liquids. At the end of 2023, I spent a semester abroad in Turku, Finland.

Computational Study of Porous Organic Polymers with Nitrogen-Rich Functionalities for Selective CO_2 Adsorption

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Due to an increase in carbon dioxide levels in nature, there has been a need for efficient and highly selective CO_2 capture materials. One of the promising candidates are porous organic polymers with nitrogen-rich functionalities, whose CO_2 adsorption abilities can be fine-tuned by examination of different building blocks (triphenyl substituted amine, pyridine, benzene and 1,3,5–triazine), nitrogen nitrogen linkages (azo, azoxy and azodioxy) and linear spacers (phenyl and biphenyl).[1] A part of this research was done computationally, where said functionalities were connected into 2D frameworks. The stability of the crystal structures at different neighbouring stacking configurations was examined computationally using periodic DFT methods in the CRYSTAL17 program. Optimized structures were subjected to grand-canonical Monte Carlo (GCMC) simulations in the RASPA program and adsorption isotherms were compared. Using the VTK program, the distribution of CO_2 and N_2 molecules inside

examined structures was visualized and the given data was compared with the results of the

electrostatic potential analysis. By combining an insight into local binding sites and GCMC methods, one can obtain a lot of information about the adsorption properties of porous material. With the given results, periodic DFT calculations and GCMC simulations can be a guide for the design of new functional materials by predicting promising candidates in the synthesis of covalent organic polymers with enhanced CO2 adsorption properties.[2]

This work has been fully supported by Croatian Science Foundation under project IP-2020-02-4467.

Literature

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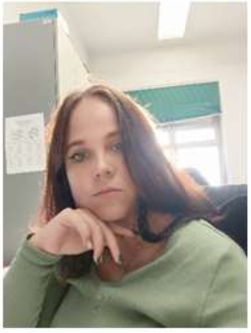

Biography

Born and living in Croatia, I, Tea Frey, graduated in chemistry 2023, majoring in organic and analytical chemistry, at the Faculty of Science, University of Zagreb, Croatia. Under the mentorship of Ivan Kodrin, I have published 2 works and won 2 rewards in the field of computational chemistry of periodical crystal organic structures. I am currently working at the Division of Organic Chemistry as an assistant.

Green Catalysis for Biomass-Derived Heterocycles: Solvent-Free Oxidation of Linalool Using Polyoxometalates

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Among the 12 principles of Green Chemistry, catalysis is fundamental to economic development and growth of chemical industry. [1] It is essential that products of interest can be produced under environmentally friendly conditions, particularly from biomass. In this study, we focused on two heterocycles with potential medicinal applications,[2] referred here as furanoid and pyranoid. These compounds are traditionally synthesized through "non-green" methods that generate significant amounts of waste and require large volumes of solvent.[3] However, recent approaches have explored the oxidation of linalool (L), a biomass-derived substrate.[4] Motivated by environmental and societal concerns, these processes demonstrated activity without the use of organic solvents, employing complexes with tridentate ligands or polyoxometalates (POMs), representing a step toward cleaner synthesis.[5–9] Here in, the oxidation of linalool with the help of "green" benign oxidants and solvent-free conditions, used homogeneous and heterogeneous catalytic systems based on polyoxometalates that could be grafted on silica supports. The synthesis of supported catalysts and their performance under various reaction conditions will be discussed.

Literature

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Biography

Ali holds Bachelor and Master 1 degree in Physical Chemistry from the Lebanese University in Beirut. He further specialized with a Master 2 in Synthesis, Catalysis, and Sustainable Chemistry from Claude Bernard University Lyon 1. Currently, he is pursuing a PhD in the same domain at the Laboratoire de Chimie de Coordination (LCC) in Castres, France, where his research focuses on sustainable chemistry through innovative homogenous and heterogeneous catalytic processes. He is involved in the SOSOPRO and SusPolMoV projects between France and Croatia.

Molecular dynamics of solvent effects on ions, ion pairs, and ion aggregates

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Theoretical models of ion effects have a long tradition in Theoretical Physical Chemistry, where force-field based MD simulations are widely used. For small ions, for example alkali metal ions or halides in water, some key principles have been understood like the concepts of strong vs. weak hydration or the ordering of these ions in the Hofmeister series.

In recent years a new class of ions has been the topic of interest: ions that are much larger in size and are at the same time multiply charged. These “nanoions” have special properties in the way they bind to interfaces and solutes. For this class of ions, the theoretical understanding is much less developed. In this talk, we will discuss some of the key principles of ion specificity and present simulations of simple nanometer sized spherical ions[1].

Next we will discuss solvation properties of ion pairs and aggregates in organic solvents, that are important in ion pair catalysis. These comprise a chiral phosphoric acid (CPA) and an imin. We will discuss binding motifs observed in dichloromethane.

Literature

[1] P. Dullinger; D. Horinek. *J. Am. Chem. Soc.* **2023** (145) 24922.

Biography

2000 Ph.D. in Physical Chemistry, University of Regensburg

2001-2005 Postdoc, University of Colorado, Boulder, USA, Czech Acad. of Science, Prague

2010 Habilitation inTheoretical Physics, Technical University of Munich

Since 2010 Professor of Physical Chemistry, University of Regensburg

Mechanochemical Synthesis and Crystal Structures of the Alkali Metal Magnesium Chalcogenides

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New potential sodium-ion conductors are in the focus of this paper. We report on the synthesis and impedance spectroscopic investigation of new sodium magnesium chalcogenides.

The literature known material Na_6MgS_4 and the heavier homologous compounds Na_6MgSe_4 and Na_6MgTe_4 were prepared via high-temperature solid-state reactions from the elements. All three compounds crystallize isostructural to Na_6ZnO_4[2] in the non-centrosymmetric space group $P6_3mc$ (No. 186). The crystal structures of Na_6MgSe_4 and Na_6MgTe_4 were determined by single-crystal X-ray diffraction and confirmed by powder X-ray diffraction.

Na_6MgS_4 crystallizes with cell parameters a = 9.0236(1) Å, c = 6.9499(1) Å and an unit cell volume V = 490.082(7) Å^3, with Z = 2. For Na_6MgSe_4 the lattice parameters are a = 9.4162(2) Å, c = 7.2285(1) Å, and V = 555.05(3) Å^3 with Z = 2, while Na_6MgTe_4 exhibits parameters of a = 10.1091(8) Å, c = 7.7044(5) Å and V = 681.86(12) Å^3, also with Z = 2. These compounds form a wurtzite-like three-dimensional framework consisting of corner-sharing MgQ_4 (Q = S, Se, Te) and NaQ_4 tetrahedra. Tunnels parallel to the c-axis accommodate octahedrally coordinated sodium atoms in 3/4 of the available sites.

The ionic conductivity of Na_6MgS_4 at 40 °C is 1.4×10^{-10} S cm^{-1} and 7.5×10^{-4} S cm^{-1} at 300 °C (E_A = 0.78 eV). In contrast, Na_6MgSe_4 and Na_6MgTe_4 exhibit no measurable ionic conductivity.

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Huf Elisabeth Poster presentation

Biography

B.Sc. Chemistry at University of Regensburg - Okt. 2016 – Nov. 2020

M.Sc. Chemistry at University of Regensburg - Okt. 2020 – Sept. 2022

PhD Student at University of Regensburg - since Dec. 2022

Analysis of Lanthanide Ion Sorption On Calcium Alginate-Encapsulated Iron Nanoparticles Using Inductively Coupled Plasma-Mass Spectrometry (Icp-Ms)

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Lanthanides play a crucial role in the development of advanced technologies, but their growing use may pose risks to the environment and drinking water supplies. Consequently, it is essential to find new methods for extracting these elements from aqueous environments. This study introduces a novel approach utilizing encapsulated zero-valent iron nanoparticles (nZVI). The nZVI particles were modified with pyridine-2,6-dicarboxylic acid and embedded within an alginate hydrogel, and were employed for the removal of lanthanum, europium, gadolinium, and dysprosium from water. Pyridine-2,6-dicarboxylic acid forms stable complexes with lanthanides, while the hydrogel encapsulation enhances the mobility of the nanoparticles and improves their resistance to agglomeration and oxidation, compared to bare nZVI.[1,2] The sorption efficiency was evaluated for individual lanthanide solutions as well as for a mixture of lanthanides using inductively coupled plasma-mass spectrometry (ICP-MS). When compared to unmodified nZVI, the functionalized nanoparticles demonstrated better performance in adsorbing a mixture of the four lanthanides, whereas the neutral nZVI showed higher efficacy in adsorbing the individual lanthanides from water.

Literature

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Biography

Nikolina Ilić completed her Undergraduate Degree in Chemistry (2020) and Graduate Degree in Chemistry (2022) at the Faculty of Science, University of Zagreb, defending her thesis under the title " Electron microscopy characterization of iron nanoparticles used for sorption of selected lanthanides". Since July 2023, she has been employed as an expert associate at the Division of Analytical Chemistry at the Department of Chemistry of the Faculty of Science, University of Zagreb. She participates in the Analytical Chemistry Practice courses 1 and 2 at the Undergraduate Study in Chemistry and the Instrumental Analysis 1 and Higher laboratory in analytical chemistry 1 courses at the Graduate Study in Chemistry. In 2023, she enrolled in Doctoral study in Chemistry (major: Analytical Chemistry). She specializes in analytical atomic spectrometry based on plasma sources, focusing on research of iron nanoparticles. She participated in 6 scientific conferences with 2 oral presentations and 4 poster presentations.

Influence of An External Electric Field On Silica Nanoparticles

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The mineral/aqueous electrolyte interfaces are of critical importance in many technological and environmental processes. The mineral surface is a site for such reactions as adsorption, ion exchange, surface dissolution, and crystallization. The behavior of metal oxides in aqueous solution, including silica (SiO_2), is determined by various factors, such as pH, ionic strength, and the nature of background electrolyte.[1] The surface properties of SiO_2 are key to its performance in these settings. Depending on pH, the surface silanol groups (Si-OH) either protonate or deprotonate, which can directly have an impact on how silica interacts with other species in solution.[2] Widely used methods for studying surface properties and behavior of nanoparticles in suspensions are based on electrophoresis, which examines the motion of colloidal particles under an electric field. Used electric field could also influence the behavior of silica through aggregation or dissolution of the nanoparticles. To understand this better, this study focuses on the impact of such fields on silica nanoparticles by observing the aggregation of SiO_2 particles through dynamic light scattering (DLS) and electrokinetic potential measurements using electrophoretic light scattering (ELS).[3] Additionally, the dissolution of silica, an essential aspect of its behavior in suspensions, is monitored. Silica dissolution is predominantly pH-dependent, leading to the formation of silicic acid, which can further interact with molybdate ions to form a complex that absorbs visible light. This allows the quantification of dissolved silica via UV-Vis spectrophotometry.[4] The effect of formed silicic acid on the electrokinetic potential of SiO_2 was studied. The electrokinetic potential of silica nanoparticles in sodium chloride and silicic acid solutions was measured in a wide pH range. The given results have been intended to give a more complete understanding of changes in electrokinetic potential and particle size of SiO_2 under different ionic strengths, types of background electrolyte, and pH conditions. This study, therefore, aims to assess how an external electric field affects the surface properties and reactions of colloidal silica, especially considering its potential impact on the accuracy of electrophoresis-based characterization techniques. By correlating the electrokinetic behavior with particle size changes and dissolution under varying conditions, the research explains the reliability and precision in characterizing colloidal silica in the presence of external influences.

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Biography

I am a research assistant at the Divisions of Analytical and Physical Chemistry, Department of Chemistry, Faculty of Science in Zagreb (Croatia). My teaching responsibilities involve leading laboratory exercises in analytical and physical chemistry courses. Research that I am focused on includes colloidal and interfacial chemistry, analytical methods for nanoparticle characterization, and vibrational spectroscopy. I enjoy spending my free time in good company and watching a good series or an interesting film.

Kalkhof Stefan Oral presentation

Guiding Biomaterial Design through the Power of Omics Technologies

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Bioactive, bioresorbable, and bioresponsive biomaterials exhibit significant potential in biomedical engineering. By integrating diverse materials, incorporating bioactive components with controlled release, and utilizing flexible manufacturing techniques such as 3D printing, highly adaptable solutions can be generated. However, a systematic design and optimization of biomaterials require thorough characterization of their properties, efficacy, degradation rates, and molecular and cellular interactions.[1]

In our research, we tackle central questions, including: How does the material affect the healing process? Which cells and proteins interact with it? How quickly are drugs released? What additional factors may serve as effective active components? How can we predict the outcomes of biomaterial modifications?

We employ mass spectrometry based approaches —specifically proteomics and metabolomics, as well as structural, imaging, and protein interaction analyses—that facilitate comprehensive evaluations in cellular and preclinical models. Using extracellular matrix-inspired biomaterials made from collagens and modified glycosaminoglycans as one[2-4] and 3D printed modified PCL scaffolds as a second example[5-7], two journeys will be presented reaching from the initial biomaterial concept through the optimization of material design to successful preclinical testing in small and large animal models.

Kalkhof Stefan Oral presentation

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Biography

Prof. Dr. Stefan Kalkhof has been a Professor of Instrumental Bioanalysis since 2015 and is one of the founders of the Coburg Institute for Bioanalysis. He also serves as the speaker for the "One Health" research focus at Coburg University. His research centers on developing therapeutic approaches through the application of bioactive, bioresorbable biomaterials. His team focuses on creating mass spectrometric analytical methods for identifying and investigating the efficacy and safety of therapeutic targets and bioactive substances released from biomaterials. The methodological work encompasses both in vitro and in vivo studies aimed at the structural elucidation of individual proteins, characterization of protein-drug and protein-biomaterial interactions, and exploration of mode-of-actions and pathomechanisms. Prof. Kalkhof is the project leader for several important research initiatives, including DFG Transregio 67, BMBF projects such as SyMBoD, reGAG, and CIMD, as well as the EU Pathfinder project ISOS. As the head of the Proteomics Unit and a member of the "Advanced Analytics" technology platform at the Fraunhofer Institute for Cell Therapy and Immunology (IZI), he has access to cutting-edge equipment for preclinical and clinical studies, including modern mass spectrometers for proteomics and metabolomics, which are also utilized in various industry collaboration projects.

Application of mass spectrometry in characterization of drug:β-cyclodextrin systems

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Cyclodextrins are cyclic oligosaccharides containing six (α-CD), seven (β-CD), eight (γ-CD), or more (α-1,4-)-linked D-glucopyranose units. Their interesting properties offer the potential for CDs to enhance solubility and improve the stability of active pharmaceutical ingredients through the formation of host:guest inclusion complexes via non-covalent interactions.[1] The knowledge of the non-covalent molecular interactions that occur in supramolecular systems is the basis of their applications. Thorough analytical characterization of cyclodextrin complexes is of fundamental importance to provide adequate support in selecting the most suitable cyclodextrin for each guest molecule. The full analytical characterization of CD inclusion complexes is not a simple task and involves the use of several analytical techniques, whose results must be combined and evaluated together. There has been growing interest in advancing efficient and reliable analytical methods that assist with elucidating CD host:guest drug complexation. One of the techniques with an increasing application in this field is mass spectrometry (MS). The use of MS together with soft ionization techniques such as electrospray to investigate drug:CD inclusion complexes in gas-phase is recently becoming popular because this technique can provide information about non-covalent gaseous ion, structural determinations, stoichiometry of the inclusion complexes, reactivity in gas-phase and gas-phase thermochemical data.[2] Tandem MS experiments performed on ions of drug:CD complexes have already been used to compare the stability of their gas-phase conformations which can potentially reflect their solution-phase stability. Here, we present our recent results on exploring host:guest inclusion complexes of various drugs such as praziquantel[3], nabumetone[4], loratadine[5], and cinnarizine with natural β-CD and its derivatives (namely randomly methylated β-CD, hydroxypropyl-β-CD, and sulfobutylether sodium salt β-CD). Apart from the structural determination of host:guest inclusion complexes in gas-phase by mass spectrometry, we are focused on investigating the stability of various drugs in potential cyclodextrin pharmaceutical formulations with improved properties. In such studies, liquid chromatography – high-resolution mass spectrometry is a technique of choice due to its sensitivity and potential to provide unequivocal structural characterization of degradation products observed during forced degradation studies and long-term or accelerated stability testing.

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Biography

David Klarić was born in 1991 in Mostar (Bosnia and Herzegovina). After completing his undergraduate studies in biology and chemistry in 2014, he trained professionally for seven months in the United Kingdom, after which he enrolled in graduate studies at the Chemistry Department of the Faculty of Science, University of Zagreb in 2015. He graduated in 2018 and defended his doctoral dissertation in 2024. As a scholarship holder of the “Central European Exchange Programme for University Studies”, he trained for five months at the Universities of Pécs, Budapest, Warsaw, and Graz. Since 2019, he has been employed as an assistant at the Department of Analytical Chemistry of the Chemistry Department of the home faculty. His scientific research involves the investigation of non-covalent interactions of poorly soluble drugs and cyclodextrins in solution and in the solid state. He published several scientific papers, participated in international and domestic meetings, and gave invited lectures.

Better Organic Synthesis with Light

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Light is an ideal reagent for organic synthesis. It provides energy to overcome activation barriers of reactions or even enable endothermic transformations. Photons can be used in large excess to drive a reaction to completion, but they will leave no trace. Visible or UV-A light is safe and non-toxic and easily generated with modern light sources, such as LEDs. The last two decades have seen the development of many synthetic methods that use sensitized or direct photochemistry to enable organic reactions at milder conditions, but also open new reaction pathways which are impossible in thermal chemistry.[1]

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Biography

Prof. Burkhard König's scientific work is centered on physical-organic chemistry and photochemistry. As one of the pioneers of chemical photocatalysis, he has significantly developed the field of light-driven organic synthesis in the past 20 years. He is one of the leading minds in this active research area in Germany and internationally. His contributions to the research area are ground-breaking and open new research directions. Even before the methodology of photocatalysis received greater attention in synthetic chemistry, work by the König group on flavin photocatalysis began around 2000. The group reported the first photocatalytic variant of the Meerwein arylation and the first enantioselective heterogeneous photocatalysis with visible light. They introduced the concept of consecutive photo-induced electron transfer (conPET), established the redox-neutral utilization of carbon dioxide in synthesis via photogenerated carbanions, and used organic semiconductors and excited anions in photocatalysis. Recent contributions focus on dynamic photo-nickel catalysis and synthetic photochemistry at the water-oil interface. All projects combine synthetic methodology development with mechanistic investigations to pave the way for predictable applications in synthetic chemistry and industrial production processes. In close collaboration with groups from molecular biology, photoswitchable probes are developed that allow the reversible activation or inhibition of enzymes, GPCRs, and ion channels.

Thermodynamics of Sio$_2$ Surface Reactions: Protonation and Associations Of Sodium Ions

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Mineral/aqueous electrolyte interfaces play an important role in the environment and technology. The chemical properties of minerals, as well as the composition of aqueous medium determine the processes at the surfaces. In the case of chemically nonreactive materials, surface processes may be simple and involve only the distribution of potential determining ions between the interface and the bulk of the solution. However, at the mineral surfaces the surface complexation and adsorption of ions and molecules take place.[1] Even though many research papers on the topic have been published, calorimetric studies of such systems are rare and therefore present important contribution to the field of colloid and interfacial chemistry.[2-4]

In this work the processes that occur at the silica / aqueous solution interface are explored using the isothermal reaction calorimetry (ITC) and acid-base potentiometric titrations. With this methods enthalpy of surface protonation was determined. Furthermore, using sodium ion-selective electrode and ITC, the influence of presence of sodium cations was described. It was found that the enthalpies of protonation are independent of pH and ionic strength, while those related to sodium ion association are influenced by pH and the charge of the silica nanoparticle surface. Additionally, dynamic and electrophoretic light scattering were used to access the particle size, electrokinetic potential and colloidal stability.

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Biography

Karla Korade finished bachelor's degree in chemistry in 2017 and master's degree in 2019 (thesis: Synthesis and characterization of nanoparticles of different morphologies), both at Faculty of Science, University of Zagreb. She has published 3 research papers. Her research interests are colloid chemistry, surface chemistry, thermodynamics and physical chemistry of macromolecules. In her free time, she enjoys cooking, classical literature and spending time with family and friends.

Improving the Solubility of Plastic-Degrading Enzymes through Ancestral Sequence Reconstruction

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The growing concern over plastic pollution necessitates innovative biodegradation approaches,[1] particularly for biopolymers like polylactic acid (PLA).[2] In this study, we identified a novel enzyme, MGY, exhibiting PLA-degrading activity from a metagenomic database. Despite its effectiveness, the MGY enzyme suffered from low solubility and poor yield, complicating structural and functional characterization. To overcome these challenges, we utilized ancestral sequence reconstruction as a strategic design tool.[3] This approach allowed us to infer and produce ancestral enzyme variants from three distinct evolutionary nodes, all of which demonstrated significantly enhanced solubility and expression yields. Activity assays (Fig 1.) confirmed that these ancestral variants retained strong PLA-degrading activity and could be obtained in higher concentrations. This advancement facilitates downstream applications as well as detailed structural and activity studies, highlighting the potential of ancestral sequence reconstruction to enhance the use of biocatalysts for sustainable plastic degradation.

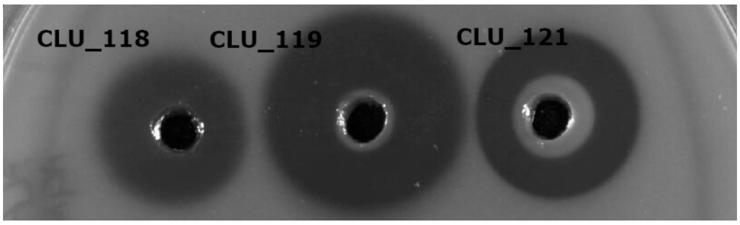

Fig. 1 All three ancestral variants of MGY enzyme show robust PLA-degrading activity.

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Biography

Aleksandra Maršavelski is an Associate Professor at the Faculty of Science, University of Zagreb (UoZ), Zagreb, Croatia. She earned her PhD in computational enzymology from UoZ in 2017. She is the author of 24 peer-reviewed papers, including 18 in Q1 and 6 in Q2 journals. Her scientific interests lie in protein chemistry, with a primary focus on studying the activity and selectivity of enzymes using computational (bio)chemistry methods alongside experimental protein chemistry techniques.

In 2023, she was awarded the WiRe Postdoc Fellowship at the University of Münster, Germany, in the group of Prof. Erich Bornberg-Bauer, for her project "Ancestral Protein Reconstruction for Developing Enzymes for Degrading Environment Polluting Bioplastics." She is currently leading the project "Enzyme Engineering for Sustainable Bioplastic Recycling," funded under the call: Research Projects for Young Researchers, as part of The National Recovery and Resilience Plan through Next Generation EU (July 2023 to July 2026).

She is the Croatian representative on the Management Committee and the leader of Working Group 2, "Computational Optimization of Catalytic Properties," within COST Action CA21162 - Establishing a Pan-European Network on Computational Redesign of Enzymes (COZYME). Aleksandra Maršavelski is the founder and organizer of the FEBS Advanced Course "Computational Approaches to Understanding and Engineering Enzyme Catalysis," held biennially.

(Bio)Analytical Chemistry and Sensor Research at Regensburg University: An Overview

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The Institute of Analytical Chemistry, Chemo and Biosensors has a broad research profile and is represented by several research groups.

The focus of the Baeumner group is on the development of biosensors, miniaturized systems and nanomaterials for bioanalytical applications. Liposomes, nanofibers, and 2D graphene-like materials are developed, characterized and applied to enhance the performance of bioassays that can be used at the point-of-care or directly in-field. Signal enhancement, transduction and especially also sample preparation strategies can be ameliorated through unique properties of the nanomaterials. Furthermore, liposomes are investigated as biomimics in the study of the innate immune system. The resulting biosensors provide solutions to challenges in food safety and environmental monitoring and in clinical diagnostics, by providing simple assay processes and low limits of detection.

The Wegener lab is focused on interfacing animal/human cells (2D monolayers or 3D aggregates) with physical transducers (e.g. planar electrodes, optrodes, piezoelectric devices) to monitor the cell response during toxicological or pharmacological assays label-free and in real-time. The non-invasive nature of the measurement provides the dynamics of the cell response as a yet underestimated level of bioanalytical insight. This research direction aims to replace classical concentration-analysis by effect-analysis using biological organisms in general, and human cells in particular. Combining individual transducer principles in one device increases the information content about a given cell population and often includes invasive actuators (electroporation, electrofusion).

The Hirsch lab is dedicated to the development of nanomaterials for advanced analytical applications. We focus on the synthesis, characterization, and functionalization of these materials, aiming to harness both electrical and optical phenomena at nanoscale interfaces. The unique properties emerging at the nanoscale offer new opportunities to solve bioanalytical challenges, particularly in sensor technologies and imaging techniques. We aim to explore these novel properties to enhance sensitivity and specificity in biological detection. Our primary materials include upconverting nanoparticles, carbon nanomaterials, and metallic particles or interfaces, providing a versatile platform for innovative solutions in bioanalytical research.

The Duerkop lab synthesizes and uses (gold) nanoparticles, electrospun nanofibers, dyes, and luminescent probes (organic dyes, metal-ligand complexes and lanthanide complexes) for the development of bioanalytical assays, lateral flow assays and optical sensors. All those probes serve to quantitate biomolecules (e.g. hydrogen peroxide, amines, DNA, ions, enzymes, enzyme substrates/products, volatiles, and tumor metabolites) or determine pH. The presence of an analyte may be indicated (visibly) by color (i.e. chromogenic dyes), or read out by photometry, reflectometry, chemiluminescence or various parameters of luminescence (intensity, lifetime). By combining those techniques, we strive to enhance the information density of assays and sensor readouts.

The Matysik group specializes in the development of advanced instrumental methods for diverse applications, ranging from bioanalysis to battery research. Our work spans a variety of techniques, including capillary electrophoresis, electrochemical methods, innovative injection and detection concepts, and mass spectrometry. Our laboratories are equipped with state-of-the-art commercial instruments, as well as custom-built devices such as voltammetric measuring systems, a time-of-flight mass spectrometer, a scanning electrochemical microscope, and a compact mobile capillary electrophoresis unit. We also have systems for online coupling of electrochemistry with mass spectrometry. A key focus of our research is the hyphenation of different instrumental components to achieve more comprehensive analytical insights.

Biography

Frank-Michael Matysik is Professor of Analytical Chemistry at the University of Regensburg (Bavaria, Germany). He studied chemistry at the University of Leipzig and received his Ph.D. (1994) and “Habilitation” (2001) degrees from the University of Leipzig. From 2001 to 2008 he was “Privatdozent” for Analytical Chemistry at the same university. In 2008, he accepted the position of a professor of chemistry at the University of Regensburg where he is representing the field of instrumental analytical methods. His research interests include electroanalysis, instrumental analytical developments, electrophoretic separation techniques, mass spectrometry, hyphenated analytical systems, and miniaturized sample preparation techniques. The Matysik group has published approximately 200 research papers. For details, please visit https://go.ur.de/matysik

Quantum Crystallography as a Chemist’s Tool for Bond Analysis

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In two different examples the insights gained from complementary bond analysis from quantum crystallography into chemical bonding are highlighted. Both examples are based on the combined methods of an “experimental charge density” coming from a multipolar model (MM), [1] and an “experimental wavefunction” coming from X-ray restrained wavefunction (XRW) fitting.[2] The first example shows how the reactivity of the organometallic synthon for white phosphorus [Ni]cyclo-P3 ([Ni] = 1,2,3-trimethyl-cycplopentadienylnickel) can be explained and categorized as a metallatetrahedrane using MM and XRW.[3] Experimental frontier orbitals were able to correctly capture the reactivity of [Ni]cyclo-P3 which was not able by previous DFT studies.[4] In the second example the ylid/ylene and carbonyl/carbonylate equilibrium in WYLID is investigated as a contribution to a long ongoing debate in the quantum crystallography community about this system. This compound is of particular interest as it closely resembles YLID, the most measured single-crystal structure in the world. [5,6]

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Biography

I am Florian Meurer, a PhD. student at the University of Regensburg in the crystallographic group of Dr. Michael Bodensteiner. I did my BSc as well as MSc degrees in Regensburg on the topic of the crystalline sponge method and the refinement of anomalous dispersion parameters in single-crystal diffraction experiments, respectively. For my PhD project on anomalous dispersion, radiation damage and different wavelengths used for the crystalline sponge method I was able to work for five months at the Rossendorf-Beamline of the European Synchrotron (ESRF) in Grenoble, France. I am currently chair of the German Young Crystallographers and want to help crystallography to “be carried on” by future generations.

A Time-Resolved Look on Photochemical Processes for which Adjacent Molecules Play a Crucial Role

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In a study on supramolecular hosts that can encapsulate small guest molecules, ultrafast spectroscopy was employed to address how the guest alters the photoswitching characteristics of the cage. For this, the impacts of three disparate guest compounds on ring-opening or ring-closure of a dithienylethene (DTE) ligand in a photoswitchable DTE-based coordination cage are juxtaposed. It is shown that the guest can modulate both the outcome and timescale of the cage's photodynamics.[1]

Interaction with an adjacent molecule can also be employed for deracemization. The substrate binds to a chiral photocatalyst by two-point hydrogen bonding, i.e., a pre-complexation exists when the catalyst is excited by light. Two criteria have to be met for the reaction to work efficiently: First, light absorption triggers a transfer process that works better (or exclusively) for one of the enantiomers. Second, an achiral intermediate has to be formed whose lifetime exceeds that of the complex, so that the subsequent reformation of the chiral substrate is not enantioselective. For the deracemization of hydantoins,[2] a hydrogen-atom transfer (HAT) to the chiral benzophenone catalyst occurs which is only possible for one hydantoin enantiomer due to steric reasons. The back HAT yields an achiral enol intermediate which reforms the hydantoin in a non-enantioselective way in an enol-keto tautomerization.

The contributions of R.J. Kutta, R.J. Li, S. Juber, E. Benchimol, L.V. Schäfer, G.H. Clever, J. Großkopf, N. van Staalduinen, A. Seitz, P. Pracht, S. Breitenlechner, C. Bannwarth, and T. Bach are highly acknowledged, as is funding by the DFG within CRC 325.

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Nuernberger Patrick Oral presentation

Biography

Patrick Nuernberger received his Doctorate from the Univ of Würzburg in 2007. He further worked at SUNY Stony Brook, Ecole Poly-technique, and Ruhr-Univ Bochum. Since 2019, he has held the Chair of Physical Chemistry at the Univ of Regensburg. His research focuses on investigating chemical reactions, catalytic processes, and dynamics induced by light with advanced time-resolved spectroscopic methods.

Self-polymerization of disulfide-containing nitrosoarenes on gold surface

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Adsorption of organic molecules on surfaces and their arrangements into self-assembled monolayers (SAMs) or multilayers provides a versatile route for developing functional materials with a wide range of applications. Aromatic C-nitroso compounds exhibit unique characteristics, such as the ability to dimerize or polymerize into azodioxides, which offers a means for the controlled fabrication of azodioxy thin films. Since the nitroso/azodioxy system displays photochromic and thermochromic behavior in the solid state, these films could be disassembled and reassembled by UV light or exposure to heat. Previous studies have shown that nitrosobenzene derivatives with sulfur headgroups form nitroso monolayers and azodioxy bilayers when adsorbed on the Au(111) surface.[1–3] High-resolution scanning tunneling microscopy (STM) images revealed hexagonal molecular patterns in the monolayers and bilayers, providing structural insights into these assemblies.[1] More recently, aromatic dinitroso derivatives were found to possess intriguing electronic properties, and their incorporation into thin films could be potentially used for the construction of organic electronic devices.[4] In our recent study, we explored the polymerization of various aromatic dinitroso compounds initiated by nitroso-terminated monolayers on Au(111) surfaces, resulting in the formation of azodioxy oligomer thin films.[5]

In this study, we synthesized new aromatic C-nitroso compounds, with or without an alkyl side chain, incorporating disulfide headgroups for adsorption on gold surface, and investigated their self-assembly on Au(111) surface using Raman spectroscopy, ellipsometry, water contact angle measurements, atomic force microscopy (AFM) and STM. The obtained results revealed the formation of azodioxy oligomer films on Au(111), and the interrelationship between the molecular and surface structural features of disulfide-containing nitrosoarenes. On-surface self-polymerization of aromatic C-nitroso derivatives with disulfide functionalities could be used for the relatively simple design of azodioxy thiolate films on gold surface with various potential applications.

Acknowledgments:

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Biography

I received my MSc degree in Chemistry from the University of Zagreb, Faculty of Science in 2021. Since 2021, I'm a PhD student working in the lab of Dr. Ivana Biljan, Associate Professor at the Faculty of Science, University of Zagreb, where one of the main research focuses is the synthesis and characterization of new aromatic C-nitroso derivatives and their self-assembly on the surfaces. My research, which I am conducting as part of my PhD thesis, is to establish guidelines for the controlled design of self-assembled azodioxy films and 2D polymers on solid surfaces and to investigate the mechanisms of their self-assembly to gain better insight into the bottom-up design of new functional organic materials with potential applications in molecular electronics.

Optimizing Sers Detection Of G-Quadruplex: Influence of Gold Colloid Stabilizing Species

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G-quadruplexes (G4) are noncanonical secondary structures formed by DNA or RNA sequences that are rich in guanine (G) bases. They result from the stacking of G-rich sequences into G-quartets, where four guanine bases bond through Hoogsteen hydrogen interactions, creating a square-like configuration. These G-quartets can stack together to form a G4 structure. G-quadruplexes have attracted considerable attention because of their distinct structural characteristics and diverse biological roles, especially in drug design[1].

Surface-enhanced Raman scattering (SERS) spectroscopy is a powerful tool for exploring the structural dynamics and stability of G-quadruplexes. SERS allows detection of molecules at very low concentrations by amplifying the Raman scattering signal due to adsorption or chemical binding of molecules to a nanostructured metal surface which enables a thorough analysis of the complex features of G-quadruplex structures[2].

This research focused on the anti-parallel G-quadruplex formed by the human telomeric sequence Tel24, stabilized by Na^+ ions, using SERS. Two distinct SERS-active substrates were used: citrate-stabilized and spermine-stabilized gold nanoparticles. Near-infrared laser excitation at a wavelength of 785 nm was utilized for the analysis. The unique SERS signatures, particularly the bands associated with the breathing vibrations of adenine (~730 cm^{-1}) and guanine (~660 cm^{-1}) aromatic rings, enabled the detection of the G4 at a concentration of 4×10^{-5} mol/L. Monitoring the relative intensities of these bands allowed observation of structural transitions from the unfolded oligonucleotide to the G4 form[3]. The spectral differences were analyzed, providing insights into the effectiveness of the SERS substrates in capturing distinct G-quadruplex formations. Notably, potential interactions between the spermine stabilizer and the G4 may have hindered the positively charged substrate's ability to detect structural changes more effectively. This was unexpected, as it was anticipated that the positively charged substrate would electrostatically attract the negatively charged oligonucleotide and strongly enhance Raman scattering. On the other hand, citrate-stabilized gold nanoparticles proved to be more effective as SERS substrate for detecting G-quadruplex formation, despite the theoretical drawback of their negative charge, which should electrostatically repel negatively charged oligonucleotide.

This research deepens our understanding of G4 structural dynamics and emphasizes the significance of selecting suitable SERS-active substrates for monitoring such changes.

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Biography

Petra Petrović, mag. chem. is a doctoral student at the University of Zagreb Faculty of Science, Department of Chemistry. Her research interests center around exploring the unique capabilities and applications of Surface-Enhanced Raman Scattering (SERS), a powerful analytical technique that enables enhanced detection and characterization of molecules at the nanoscale. Currently, her work involves utilizing SERS to detect G-quadruplex formations, aiming to enhance the understanding of its structure and interactions with small organic molecules and advance the field of SERS by contributing novel insights in the structural changes of G-quadruplexes and their dynamics. Petra published one peer-reviewed paper titled "SERS evidence of urea-disordered G-quadruplex structure" in Journal of Raman Spectroscopy (https://doi.org/10.1002/jrs.6586). She has also been awarded two mobility grants from University of Zagreb for attending conferences in Lisbon, Portugal and Rome, Italy; an ICORS 2024 Student grant, and a CEEPUS mobility grant for Summer School in Ljubljana, Slovenia. She presented her work at two international conferences and four domestic conferences. Additionally, Petra has served as a member of the Organizing committee for 7th PhD Student Symposium and as the Organizing committee Chair for 8th PhD Student Symposium in Zagreb, Croatia, gaining valuable experience in academic event coordination.

Preparation and characterization of binary systems of loratadine and β-cyclodextrin and its derivatives in solid state

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Cyclodextrins (CDs) are known for their ability to form inclusion complexes with various molecules affecting their physico-chemical properties. Therefore, they are of great interest in pharmaceutical industry in developing new strategies for improving the solubility of low soluble drugs, such as loratadine (LOR), an antihistaminic drug with low solubility and high permeability.[1,2] Mechanochemical activation is a fast and efficient method for preparation of inclusion complexes in solid state that does not require use of organic solvents.[1]

In this work we present a method of preparation of inclusion complexes of LOR and β-CD and its hydroxypropylated (HP-β-CD), randomly methylated (RM-β-CD) and alkysulfonated (SBE-β-CD) derivatives by grinding in vibrational high energy ball mill. Binary systems were prepared in stoichiometric ratios 1:1 and 1:2. Method of grinding was optimized in terms of number of milling balls, vibrational frequency and sample mass. Efficiency of grinding was determined by differential scanning calorimetry by calculating decrease in crystal fraction of loratadine in the sample. The complexes were also prepared by conventional method, spray drying, and the results of both methods were compared.

This work was supported by Croatian Science Foundation (project IP-2022-10-6033).

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Pocrnić Marijana Poster presentation

Biography

Marijana Pocrnić graduated in 2015 at the Department of Chemistry, Faculty of Science, University of Zagreb. From 2017 she is employed at the Division of Analytical Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb. In academic year 2018/2019 she enrolled in Doctoral studies in Chemistry. She was awarded 4 CEEPUS scholarships for a one month stay at the Universities of Prague, Pecs and Budapest. Her scientific research involves development and validation of liquid chromatography and liquid chromatography coupled with high resolution mass spectrometry methods, structural characterization of degradation products and investigation of interactions of cyclodextrins and drugs with low solubility in solution and solid state. She published 12 scientific articles and participated in over 10 international and domestic meetings with poster or oral presentations.

Polyoxometalate-Supported Silica-PEI Nanocomposites for Efficient Catalytic Valorization of D-Fructose

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The growing demand for renewable and sustainable chemical sources has made fructose valorization a critical area of research.[1] Polyoxometalates (POMs), a class of inorganic metal oxide clusters, have gained prominence as catalysts[2,3] in the conversion of carbohydrates into key platform chemicals like 5-hydroxymethylfurfural (HMF) and diformylfuran (DFF). In this study, we explored the catalytic performance of anionic POMs ($[PMo_{12}O_{40}]^{n-}$) supported on two types of Silica-PEI nanocomposites—mesoporous SBA-15 and non-porous Stöber silica—during alcohol oxidation and D-fructose valorization. Solid-state techniques (^{31}P NMR, UV-Vis-NIR, EPR) revealed a photo-induced reduction of Mo6+ to Mo^{5+}, demonstrating a strong interaction between the POMs and amino groups on the PEI polymer. The two nanocomposites showed distinct catalytic behavior. Stöber-[PEI][POM] reached an 80% yield of HMF after 1 hour at 150°C and 50% DFF after 5 hours. Conversely, SBA-15-[PEI][POM] achieved a higher HMF yield (92%) but only a 6% DFF yield, suggesting that the mesoporous structure may hinder further oxidation due to confinement effects. Mechanistic studies confirmed the POM oxidation-reduction cycle (Mo^{6+}/Mo^{5+}) driven by fructose itself. These results highlight the potential of POM@APS catalysts in sustainable fructose valorization, offering promising pathways for renewable chemical production.

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Biography

Israel T. Pulido-Díaz is a PhD candidate in Organometallic and Coordination Chemistry, conducting research through a bilateral collaboration between the National Autonomous University of Mexico (UNAM) and Université Toulouse III: Paul Sabatier. His work focuses on sustainable catalysis, particularly on development of hybrid materials and metal complexes for catalytic processes aimed at biomass valorization, CO_2 utilization and green chemistry applications. Under the mentorship of Prof. Itzel Guerrero-Ríos and Prof. Dominique Agustin, Israel made significant contributions to the field of supported metal catalysts or metal clusters.

Israel's experience spans both homogeneous and heterogeneous catalysis, with expertise in spectroscopic techniques, reaction setup, and reactor design. His international research experience, supported by the IFAL Excellence Scholarship, has cultivated his leadership, adaptability, and commitment to addressing global environmental challenges through innovative chemical research. He aims to continue his work in catalytic methodologies that minimize environmental impact and optimize raw material use.

Alice's Adventures in PhysOrg Land

Elias Harrer,[1] Maximilian Schimpf,[1] Hannes Sterzel,[1] Daniel Schmidhuber,[1]
Julia Rehbein[1]

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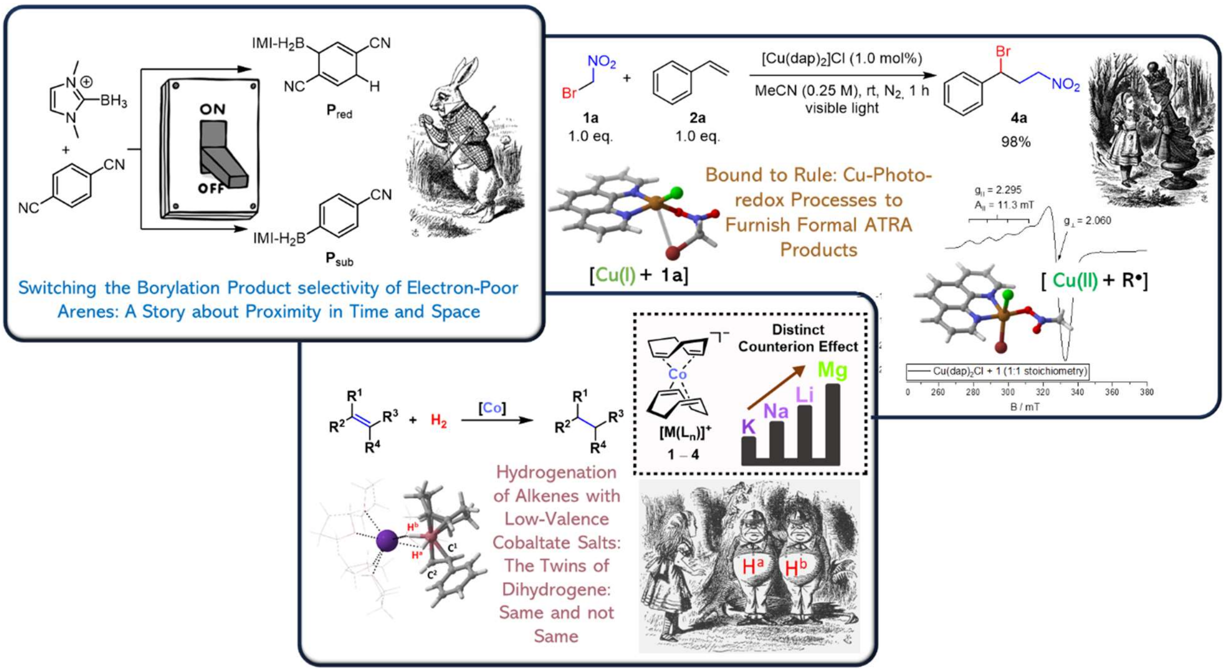
At the heart of our research is the detailed understanding of how transformations work including aspects beyond the conventional pathways defined by stationary points on the potential energy surface. This approach of going "beyond the looking glass" most often provide surprising results and help improving synthetic methods. So, how we look beyond the mirror glass? By a combination of sophisticated tools ranging from DFT- and post-HF calculations, BOMD and FF-MD simulations, EPR and pump-probe experiments, as well as classical methods like kinetics and isotopic labelling.



Here we will present short stories on how reactivity of key intermediates can be modulated by proximity effects, which may invoked by be ionic interactions in close-contact ion-pairs, ligand exchange phenomena at transition metal centers prior of after light activation, but also by timing elementary steps and steering the evolution of key intermediates in time and space.

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Biography

I was trained as a chemist at the TU Dresden (2000-2005), pursued my PhD with Prof. Martin Hiersemann at TU Dortmund (2005-2009) on asymmetric catalysis of the Gosteli-Claisen rearrangement that I could finish with the highest honours. My postdoctoral stay I could spend with Barry K. Carpenter (2009-2012) at Cardiff University working on reaction dynamic effects. My independent career started with a FCI-habilitation stipend and then as a Emmy-Noether group leader (2012-2017) at the UHH (Hamburg) dedicated to identifying radical pathways ins NHC-catalysis and dynamic effects in cationic rearrangement. I was appointed as a W2 professor in October 2017 at the UR (Regensburg) whilst declining an offer at Kaiserslautern. Our current research topics are located within the field of modern physical organic chemistry: deciphering mechanisms in (photo)catalysis, modulating bond reorganization within the boundaries of homolytic to heterolytic processes and using strain energy in meta-stable states to drive reactions of noncovalently bound substrates.

Reiser Oliver Oral presentation

Turning Hay to Gold: Catalytic Conversion of Non-Edible Renewable Resources Towards Value-Added Products

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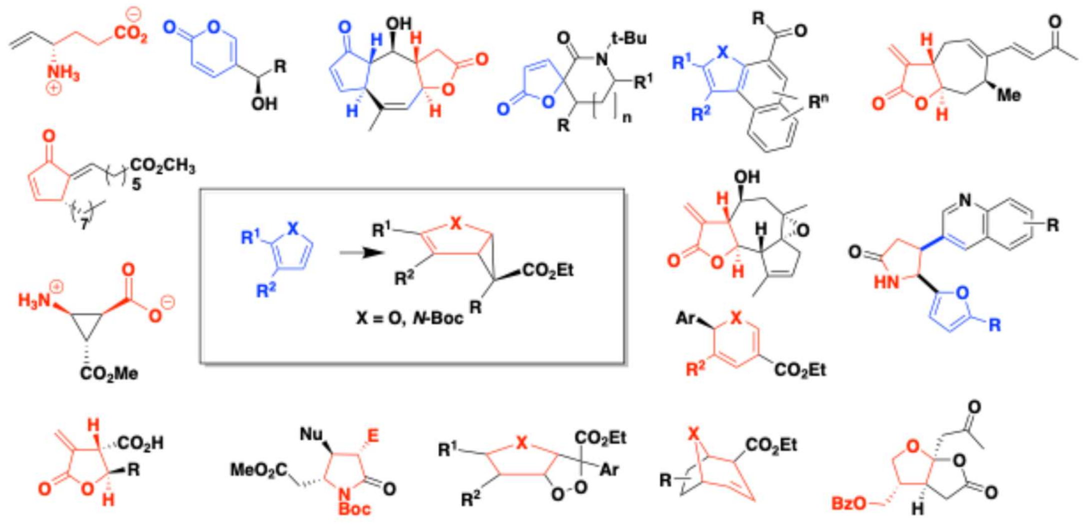
Pyrroles and furans represent readily available bulk chemicals derived from non-edible, renewable resources. Focusing on asymmetric transition metal and visible light photoredox catalysis, we are developing strategies to rapidly convert such starting materials into novel heterocyclic and carbocyclic scaffolds related to natural products or drugs.



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Biography

Oliver Reiser studied chemistry at the Universities of Hamburg, Jerusalem, and Los Angeles (UCLA) and obtained his Ph.D. in 1989 with Prof. Dr. Armin de Meijere. He spent 2.5 years as a postdoctoral fellow with Dr. R. Miller, IBM Research Center, San Jose, USA, and with Prof. Dr. D. A. Evans, Harvard University, Cambridge, USA. In 1992 he moved to the University of Göttingen as an Assistant Professor, and in 1996, he moved to the University of Stuttgart as an Associate Professor. Since 1997, he has been a Professor of Organic Chemistry at the University of Regensburg, having served as Vice President and currently as Dean responsible for Research. His group’s research interests are focused on developing sustainable methodologies for converting renewable resources towards value-added compounds.

Corrosion at Al/Au wire bonds

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This project is about corrosion and improving the reliability of integrated circuit devices in humid environment. The research focuses on the corrosion at wire bonds and aims to understand how wire composition can influence reliability. The corrosion of wire bonds occurs at the intermetallic phases formed during bonding between a metal wire (Au, Cu) and an aluminum bond pad.[1] While their corrosion is often described in literature, there is no detailed understanding how intermetallic phases, and their dopants behave during corrosion.

To gain further insight in this topic, we synthesized relevant intermetallic phases and alloys with common dopants such as Pd, Pt and Cu and investigated their corrosion properties by electrochemical measurements. This allows to determine the readiness to corrode (E_{corr}) and the speed of corrosion (j_{corr}). The poster describes the process involved in obtaining said corrosion properties, which enabled us to understand the corrosion process at Al/Au wire bonds. The results are currently prepared for publishing. Further work on the corrosion of Al/Cu wire bonds is planned.

Literature

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Rosenhammer Martin

Poster presentation

Biography

B.Sc. Chemistry at University of Regensburg - Oct. 2017 – Nov. 2020

M.Sc. Chemistry at University of Regensburg - Oct. 2020 – Sept. 2022

PhD Student at University of Regensburg - since Dec. 2022

Dynamic Structural Properties of Molybdenum Schiff Base Complexes: Synthesis, Characterization, and Applications

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Molybdenum, a transition metal recognized for its diverse oxidation states and capacity to form a wide range of complexes, plays a significant role in various applications. A particularly important class of these compounds is molybdenum Schiff base complexes, formed through the coordination of molybdenum with Schiff base ligands, which are synthesized via the condensation of primary amines and carbonyl compounds. These complexes have garnered considerable attention due to their unique catalytic and chemical behaviors.[1,2] In biological systems, molybdenum is an essential element, serving as a key component in enzymes critical to various metabolic processes.[3] Industrially, molybdenum-based complexes are widely employed in processes like petroleum refining and chemical production, where they are prized for their catalytic functions in reactions such as oxidation, hydrogenation, and olefin metathesis—key transformations in chemical synthesis.[2,4] Additionally, molybdenum complexes are increasingly important in materials science, contributing to the development of advanced materials with specialized structural and electronic characteristics. These materials play pivotal roles in fields such as energy conversion and environmental protection, enhancing the efficiency of energy devices and aiding in pollutant removal.[2,5]

In this study, we synthesized a Schiff base ligand through the condensation reaction of salicylaldehyde and oxalyldihydrazide. The ligand was then coordinated to the $[MoO_2]^{2+}$ core, yielding the complex $[Mo_2O_4(L)(MeOH)_2]\cdot 2H_2O$, in methanol. To investigate the effects of solvent exchange and vapor coordination, the complex was exposed to vapors of water, methanol, ethanol, and propanol. This exposure led to desolvation and the replacement of coordinated methanol molecules with vapor molecules, resulting in noticeable structural changes. Comprehensive characterization of the complex was performed using IR-ATR spectroscopy, thermogravimetric analysis (TG), and X-ray diffraction. Impedance spectroscopy (IS) further revealed structural changes induced by the solvent exchange, providing additional evidence of the complex's dynamic nature. Catalytic testing was also conducted to evaluate the complex's effectiveness in promoting oxidation reactions. In summary, this study highlights the versatility of molybdenum Schiff base complexes, showcasing their dynamic structural properties and catalytic potential, with applications ranging from industrial catalysis to material science advancements.

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Biography

Born in Zagreb, Croatia, I obtained a Bachelor’s degree in Chemistry in 2021 from the Faculty of Science, University of Zagreb. Later that year, I enrolled in the Master’s program in Analytical and Inorganic Chemistry at the same institution, completing it in 2023. My Master’s research focused on molybdenum Schiff base complexes, encompassing their synthesis and characterization. In 2023, I received an Erasmus+ grant, which allowed for a two-month research placement at IUT P. Sabatier in Castres, France, where I investigated catalytic reactions based on linalool oxidation. During my Master’s studies, I presented my findings at three international conferences and published two journal articles, with a third currently under review.

In 2024, I entered the Ph.D. program in Inorganic Chemistry at the Faculty of Science, University of Zagreb. My doctoral research focuses on the catalytic properties of molybdenum and vanadium complexes, particularly through the application of impedance spectroscopy. As part of the COST Netpore and COGITO projects, I returned to IUT P. Sabatier twice in 2024 to advance my competencies in catalytic reactions and collaborative research.

Mononuclear Copper(I) Halide based Materials exhibiting bright Cyan Luminescence

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The halocuprates(I) are a class of compounds with a large structural diversity. Due to its fully occupied d^{10} shell, the copper(I) cation allows linear, trigonal-planar or tetrahedral coordination by halide ligands. The smallest structural units in halocuprates(I) consist of linear CuX_2 dumbbells, trigonal planar CuX_3 units or CuX_4 tetrahedra (X = Cl, Br, I). The tetrahedra can be linked by corners, edges, or faces and form 0D, 1D, 2D and 3D anionic structures.[1-4] Organic cations serve as counter ions and influence the formation of the anionic structure. These compounds often emit visible light across various spectral regions upon optical excitation. Numerous studies have investigated the emission properties of halocuprates(I) and charge-neutral copper(I) halide clusters, highlighting their potential as low-priced emitter materials for LEDs and OLEDs.[5] It is essential to derive relations between their structure and photophysical properties to effectively use these materials for optical applications. Multiple electronic transitions contribute to the luminescence, such as *d*-*s* transitions, charge-transfer processes, or a combination of both, as well as other potential interactions.[6-9] A significant difficulty lies in the lack of understanding how each electronic transition contributes to the overall luminescence. Consequently, an important goal is to reduce possible interactions. Thus, mononuclear clusters such as CuX_2 CuX_3 and CuX_4 without any copper-copper interactions are in the focus of this study. Therefore, the two isotypic compounds Tetrahexylammonium-dichlorocuprate(I) $[N(C_6H_{13})_4][CuCl_2]$ and Tetrahexylammonium-dibromocuprate(I) $[N(C_6H_{13})_4][CuBr_2]$, containing $CuBr_2$ and $CuCl_2$ dumbbells were synthesized, investigated and compared in terms of their structure and photophysical properties.

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Biography

B.Sc. Chemistry at University of Regensburg	Oct. 2015 – Sep. 2019
M.Sc. Chemistry at University of Regensburg	Oct. 2019 – Nov. 2021
PhD Student at University of Regensburg	since Dec. 2021

$Rb_{10}Al_6Se_{14}$ a new ternary chalcogenoaluminate

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In the ternary systems consisting of alkali metals, triels, and chalcogens (M = Li, Na, K, Rb, Cs; Tr = B, Al, Ga, In, Tl; Q = O, S, Se, Te), numerous compounds with significant structural diversity have been characterized. The basic structural units of the anionic substructure of the *M*-*Tr*-*Q* systems are edge- and corner-linked [TrQ_4] tetrahedra, which assemble into anionic oligomeric, chain, layer, or framework structures, embedded in a cationic environment of alkali metal ions. A manyfold of compounds of the heavier elements of group 13 (Ga, In) have already been characterized by B. Krebs, H. J. Deiseroth and B. Eisenmann.[1-3] In contrast, ternary chalcogenoaluminates have been far less studied and, as a result, are the focus of this work. The novel, highly air sensitive $Rb_{10}Al_6Se_{14}$ crystallizes in transparent pale yellow blocks in the space group *C*2/*m* (no. 12) with lattice parameters a = 17.7252(2) Å, b =12.4077(1) Å, c = 9.2610(1) Å, β = 108.129(2)°, and a cell volume of V = 1951.25(4) Å^3 with Z = 2. Its crystal structure consists of large chain-like $[Al_6Se_{14}]^{10-}$ oligomeric anions made up of six edge-linked, slightly distorted [$AlSe_4$] tetrahedra.

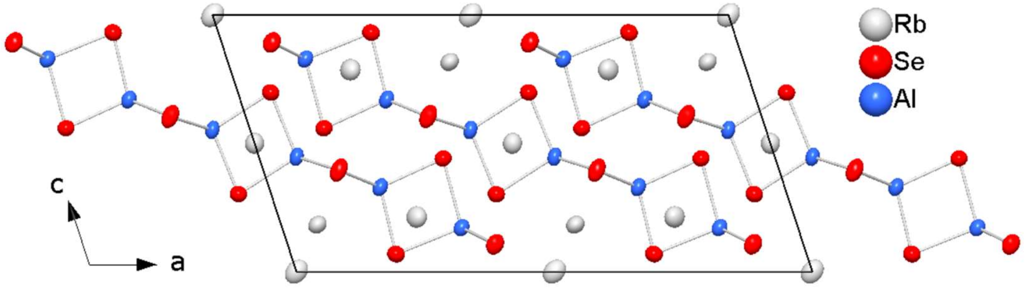

Fig. 1: Section of the crystal structure of $Rb_{10}Al_6Se_{14}$ along [010].

Literature

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Total synthesis of Penicyclone A

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Penicyclone A is a polyketide isolated from the deep-sea fungus Penicillium Sp. F32-2.[1] Its interesting structure containing a spiro[5.5]lactone core and four stereogenic centers along with the reported antimicrobial activity (MIC = 0.3 µg/mL for *S. Aureus*) prompted studies in its total synthesis. We developed the first total synthesis of penicyclone A, which was accomplished in 10 steps starting from a known D-ribose derivative.[2] The key step was a double Grignard reaction enabling the diastereoselective construction of a crucial tertiary alcohol intermediate. The synthesis also featured a tandem oxidation/cyclization for the synthesis of the lactone moiety and a photooxygenation followed by an oxidative rearrangement to introduce the enone functionality. Synthetic penicyclone A showed a discrepancy in optical rotation compared to that reported for the natural material as well as lack of antimicrobial activity. This finding prompted the synthesis of the other enantiomer which was also accomplished from D-ribose.

Literature

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[2] G. Talajić; E. Topić; J. Meštrović; N. Cindro. *J. Org. Chem*. **2022** (87) 16054–16062.

Biography

Gregor Talajić obtained his master's degree in chemistry at the University of Zagreb in 2020 with his diploma project in stereoselective Brønsted acid catalyzed methodology development. After graduating he started working at the Department of chemistry as an expert associate working on projects with the pharmaceutical industry. In 2021 he enrolled in the postgraduate program and in 2024 he defended his doctoral thesis titled "Total synthesis of penicyclone A". He is curreny working as an assistant in the Division of organic chemistry, Department of chemistry focusing on the total synthesis of antimicrobial natural products.

Copper(II) Hydrazone Complexes with Different Nuclearities

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Hydrazone complexes exhibit significant structural diversity and are widely utilized in chemistry and as biologically active substances, so they have attracted the attention of many scientists since their discovery. The properties of a particular complex depend on the type of metal and the ligands that are coordinated to the metal centre. Copper, known for its rich coordination chemistry, is primarily associated with copper(II) compounds whose coordination chemistry is dominated by ligands with nitrogen and oxygen donor atoms. This work explores the formation of copper(II) coordination complexes with hydrazone ligands. For this purpose, two ligands, pyCH=N–NH(C=O)py (HpyIZONH) and $(py)_2$CH=N–NH(C=O)py (HdipyIZONH), were prepared through the condensation of isonicotine hydrazide with the corresponding aldehyde or ketone. By reacting $Cu(NO_3)_2{\cdot}3H_2O$ with these ligands in a stoichiometry ratio of 1:1, the three-dimensional polymer $[Cu_3(\mu_3\text{-}NO_3)(pyIZONH)_3(MeOH)_3]_n(NO_3)_{2n}$ and the dinuclear discrete compound $[Cu(NO_3)(HdipyIZONH)]_2(NO_3)_2$ were obtained. In addition to reactants, the synthesis method and synthetic conditions significantly affected the nuclearity of the complex, geometry and quality of the crystal product. The molecular and crystal structures of the compounds were determined by single-crystal X-ray diffraction method. The thermal analysis indicated that these compounds are potentially explosive. To assess their stability for further synthesis, we investigated the stability of the complexes under increased pressure and temperature in dry methanol and ethanol, revealing instability under solvothermal conditions. It was found that the compounds are well soluble in water, less soluble in dimethylformamide and ethanol, and insoluble in acetonitrile.

Literature

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[4] S. Kitagawa; R. Kitaura; S. Noro. *Angew. Chem. Int. Ed.* **2004** (43) 2334 –2375.

Biography

Juraj Toplak obtained a bachelor's degree in 2021. Along with other student jobs, he gained his first experience of working in the profession while working at Pliva. Upon completion of his work, he enrolled in the graduate study of chemistry at the Department of Chemistry of the Faculty of Science. He graduated in 2024 defending his thesis entitled Symmetric Functionalization of Anderson-Type Polyoxolybdate. As a student, he volunteered in a project with polyoxomybdates at the Faculty of Science and the Ruđer Bošković Institute, for which he received an *Award* from the Department of Chemistry for scientific research work of students. His current research includes the development of hybrid organic-inorganic polyoxometalates and coordination compounds.

Achieving Molecular Complexity Via Metal-Free Domino Reactions

Svetlana B. Tsogoeva[1]

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A domino process is a powerful tool for economically and sustainably building up complex molecular architectures, drastically reducing work-up and purification steps. Recently, we developed new metal-free multi-step domino reactions and one-pot processes for waste-reducing and cost-effective preparation of versatile frameworks, which are otherwise difficult to access via traditional methods. The developed organocatalyzed methods engage simple and readily available compounds in a wide range of domino reactions to construct *e.g., azabicycles, quinazolines, quinazoline-thiohydantoins, 2,6-dicyanoanilines, o-terphenyls* and *hexaarylbenzenes* of interest for medicinal chemistry and materials science.

The *in vitro* tests against *multidrug-resistant P. falciparum* strains (Dd2 and K1), human cytomegalovirus (*HCMV*), and *multidrug-resistant* P glycoprotein-overexpressing CEM/ADR5000 leukemia cells revealed the selected domino products and some corresponding artemisinin-containing hybrid compounds as highly active agents, outperforming the clinical reference drugs. These recent results will be discussed in the talk.

Literature

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Biography

Svetlana B. Tsogoeva graduated with Distinction from *St. Petersburg State University*, where she completed her doctoral thesis supported by *Procter & Gamble*. After postdoctoral research at *Johann Wolfgang Goethe University*, Frankfurt am Main, Germany, she joined in July 2000 the *Degussa AG* Fine Chemicals Division. She was appointed in January 2002 as the first Junior Professor in Germany at the *Georg-August-University of Göttingen,* and in February 2007, as a Professor of Organic Chemistry at the *Friedrich-Alexander University of Erlangen-Nürnberg,* Germany. Her research spans topics from catalysis to medicinal chemistry. She is an Editorial/Advisory Board Member for *ACS Med. Chem. Lett*, *Scientific Reports*, *ChemPhysChem*, and a Senior Editor for *ACS Central Science*.

Homepage: https://www.chemistry.nat.fau.eu/tsogoeva-group/

The Challenges Behind Solutions: An Insight From Various Viewpoints Of Supramolecular Physical Chemists

Andrea Usenik,[1] Matija Modrušan,[1] Marija Cvetnić,[1] Katarina Leko,[1] Katarina Pičuljan,[1] Tomica Hrenar,[1] Josip Požar,[1] Nikola Cindro,[1] Vladislav Tomišić[1]

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The lecture will cover the recent investigations of the solvent effect on the thermodynamics of various host-guest complexation reactions conducted within the Supramolecular Physical Chemistry Group at the Department of Chemistry, Faculty of Science in Zagreb. The studied systems include various receptors for cationic and anionic species in solution, *e.g.* calixarenes,[1,2] as well as macrocyclic receptors (cyclodextrins and cucurbiturils) capable of binding various non-polar species in water and strongly hydrogen-bonded organic solvents.[3]

The results of combined thermodynamic, structural, and computational studies of several complexation reactions will be presented. Our comprehensive approach to correlating the obtained thermodynamic data (complex stability constants and derived reaction Gibbs energies, enthalpies and entropies) with the various host- and guest-related parameters (size, structure, functionalization, and charge), and the solvent effect will be particularly addressed.

A significant part of the lecture will be dedicated to the complexation reactions taking place in water, involving a class of glycocalixarenes designed for efficient binding of alkali metal cations in aqueous solutions.[2] Our recent investigations of the temperature effect on the inclusion of various aliphatic and aromatic guests within cyclodextrins and cucurbiturils will be addressed as well.[3] Regarding that, the influence of guest and host cavity (de)hydration on the standard thermodynamic complexation parameters will be emphasized. The results of investigations in aqueous solutions will be compared with those of the corresponding studies in structured organic solvents.

The obtained results reveal how complex and challenging it can be to explain the solvent effect on the binding ability of various hosts. With this respect, the detailed thermodynamic and structural investigations of processes taking place in various media are prerequisites for optimization of current, and targeted design of new, more efficient and selective supramolecular receptors.

Literature

[1] (a) J. Požar; M. Cvetnić; A. Usenik; N. Cindro; G. Horvat; K. Leko; M. Modrušan; V. Tomišić. *Molecules* **2022** (27) 470.

(b) K. Leko; A. Usenik; N. Cindro; M. Modrušan; J. Požar; G. Horvat; V. Stilinović; T. Hrenar; V. Tomišić. *ACS Omega* **2023** (8) 43074.

(c) M. Modrušan; N. Cindro; A. Usenik; K. Leko; L. Glazer; R. Tomaš; G. Horvat; J. Požar; V. Tomišić. *Croat. Chem. Acta* **2024** accepted for publication.

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[3] (a) K. Leko; M. Hanževački; Z. Brkljača; K. Pičuljan; R. Ribić; J. Požar. *Chem. Eur. J.* **2020** (26) 5208.

(b) A. Usenik; K. Leko; V. Petrović Peroković; Ž. Car; R. Ribić; K. Pičuljan; M. Hanževački; J. Draženović; J. Požar. *J. Mol. Liq.* **2023** (388) 122774.

(c) A. Usenik; M. Alešković; S. Roca; I. Markuš; M. Šekutor; J. Požar; *New J. Chem.* **2023** (47) 18745.

Biography

Dr. Andrea Usenik is a Research and Teaching Assistant at the Division of Physical Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb, specializing in thermodynamics of supramolecular host-guest reactions. She earned her PhD in Chemistry in 2023 from the Faculty of Science (thesis entitled *Thermodynamics of Inclusion Reactions of Amphiphilic Compounds with Cyclodextrins and Cucurbiturils*, supervisor Assoc. Prof. Josip Požar). Her current research interests include the thermodynamic and structural aspects of hydro- and solvophobically driven inclusion reactions involving cyclodextrins and cucurbiturils, as well as cation complexation by water-soluble and fluorescent calixarene derivatives. A. Usenik is the author of 7 scientific papers and has presented her work through 4 invited lectures and more than 30 poster presentations at various conferences. She was awarded several student and young researcher prizes. As the social media coordinator for the Department of Chemistry and the Croatian Chemical Society, she is passionate about science communication and promoting research visibility. Her hobbies include graphical (vector) design and conference organization, and she is currently involved in the Solutions in Chemistry conference as a conceptual founder and Conference Secretary.

Practical information

ART HOTEL
LIKE

Dear guests,

We look forward to your soon stay in our hotel and we would like to provide some basic information.

The organizer has provided your accommodation in the **Art Hotel Like, Zagreb, at the address Vlaška 44.** The reception is available 24 hours a day (info@arthotellike.hr, ++385 99 3040 393, +385 1 4616 610).

The check in is from 3:00 pm. If you arrive earlier, we will do our best to ensure a room, or in any case, you can leave your luggage at the hotel reception until check-in.

Your accommodation includes **a buffet-style breakfast,** which is served every morning from **7:00 am to 10:00 am.** For special dietary requirements, please feel free to contact the restaurant staff.

Check out is until 11:00 am.

Art hotel Like has its own vehicles for **transfers from and to the airport or any other location in the city during your stay.** For the participants of the meeting of our partner Faculty, the special transfer price for up to three passengers from or to the **airport is 30.00 EUR.** The vehicles are Mercedes Vito and can accommodate up to 7 passengers at the same time. Payment is at the hotel reception. **You can order your transfer at info@arthotellike.hr or at the mobile phone number +385 99 3040 393.**

During your stay, the reception will offer you the services of **our restaurant Obrok** in the old part of Zagreb, in our immediate vicinity. Hotel guests can enjoy meat delicacies prepared on the grill as well as "štrukli", a traditional hand-rolled dough filled with fresh cheese and cream. Hotel guests will be welcomed with a welcome drink and a 10% discount on all services.

In case of any need, feel free to contact the reception at info@arthotellike.hr or ++385 99 3040 393.

We wish you a pleasant stay in the city of Zagreb and Art Hotel Like!

Art hotel Like

Practical information

Getting to and from Zagreb Airport

If you arrive in Zagreb by plane, Zagreb Franjo Tuđman Airport is about 15km outside of the heart of Zagreb. There are several options in getting to and from Zagreb Airport, all of which are relatively straightforward.

Inexpensive Croatia Airlines airport bus

This takes you directly, without any stops, to the main bus station in central Zagreb (at Avenija Marina Drzica 4). Buses leave every half an hour (or are timed to arrive with flight arrivals at less busy periods) outside the airport terminal. Tickets, costing 8,00 EUR, can be bought from the bus driver or online at **www.plesoprijevoz.hr** where you can also find more details about the bus. The journey time is 35-40 minutes.

Taxi service

Zagreb Taxi, Bolt, Uber – all is available through the web applications.

Zagreb Taxi is the most expensive option, while Bolt and Uber will usually charge around 20-25 EUR from the airport to the Art Hotel LIKE.

Getting around Zagreb

Taxi service

Zagreb Taxi, Bolt, Uber – all is available through the web applications.

Zagreb Taxi is the most expensive option, while Bolt and Uber are quite cheap (the usual price of a ride is around 5 EUR, around city centre).

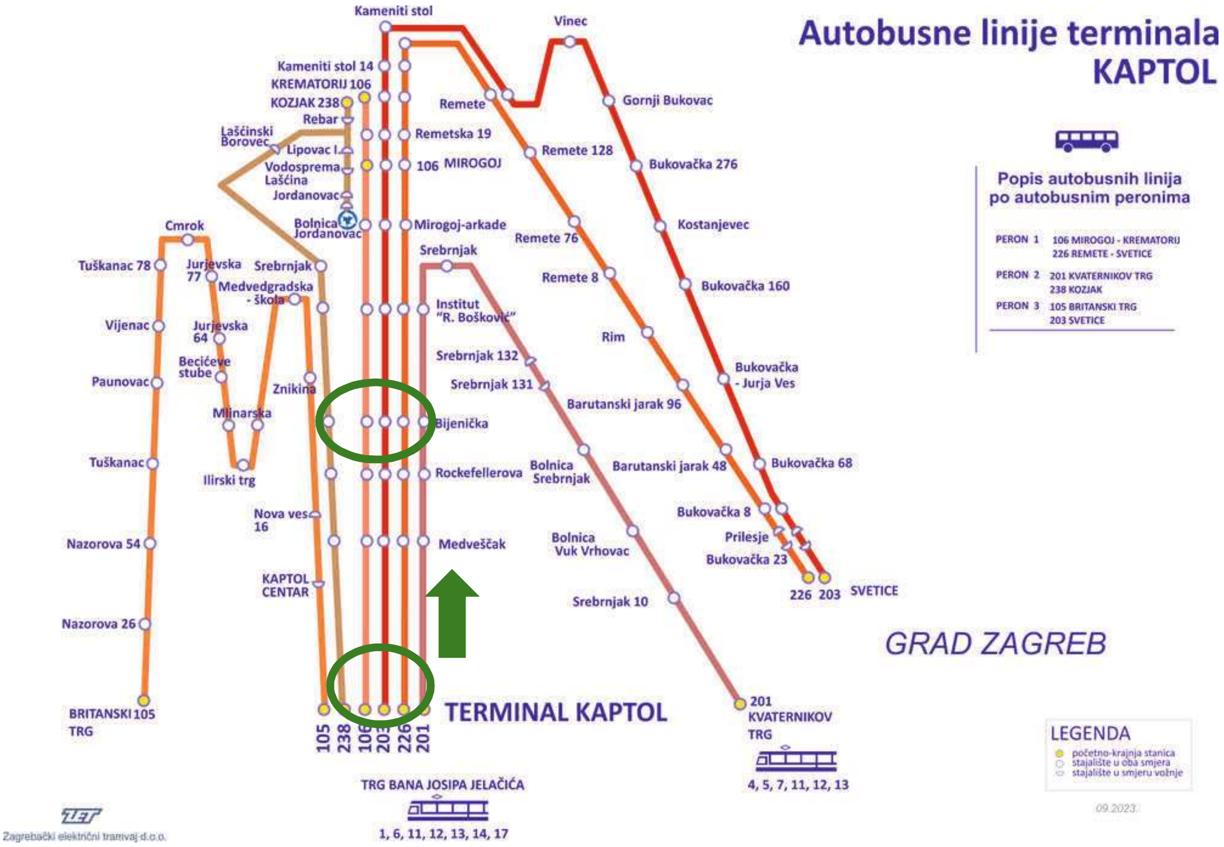
Public transportation

Numerous busses and trams are available. Ticket can be purchased in the public transport (90 min ticket is 1,99 EUR, 30 min ticket is 0,80 EUR)) or at the tobacco shop (90 min ticket is 1,33 EUR, 30 min ticket is 0,53 EUR).

Buses from Kaptol to the Faculty of Science

Lines 106, 201, 203, 226, and 238 leave Kaptol, stop at Medveščak, Rockfellerova and at Bijenička cesta you should go out and walk around 5 min to the Faculty of Science, Department of Chemistry.

Practical information



Thank you for coming!

Hvala što ste došli!