SLOVENSKI KEMIJSKI DNEVI 2025

Slovensko kemijsko društvo
Slovenian Chemical Society

17.-19. SEPTEMBER 2025

ZBORNIK POVZETKOV
BOOK OF ABSTRACTS

KONGRESNI CENTER
GRAND HOTELA
BERNARDIN, PORTOROŽ

Slovensko kemijsko društvo
Slovenian Chemical Society

Hajdrihova 19, p.p. 660
SI-1001 Ljubljana, Slovenija

Zbornik povzetkov

SLOVENSKI KEMIJSKI DNEVI 2025

Portorož-Portorose, Slovenija, 17.-19. september 2025

Uredil: Albin Pintar

Tehnična izvedba e-knjige: Taja Žgajnar, Infokart, d.o.o.

Založilo in izdalo:
Slovensko kemijsko društvo; Ljubljana, Slovenija, september 2025.

Elektronska izdaja

Datotečni format: (pdf)

URL za dostop do e-knjige: https://skd2025.chem-soc.si/
Kontakt: Slovensko kemijsko društvo, tel.: (01) 47 60 252, e-mail: chem.soc@ki.si

Cobiss ID

246603011

Kataložni zapis o publikaciji (CIP) pripravili v Narodni in univerzitetni knjižnici v Ljubljani

COBISS.SI-ID **246603011**

ISBN 978-961-95922-5-0 (PDF)

SLOVENSKI KEMIJSKI DNEVI 2025

31ST ANNUAL MEETING OF THE SLOVENIAN CHEMICAL SOCIETY

17.-19. SEPTEMBER 2025 • PORTOROŽ-PORTOROSE, SLOVENIJA

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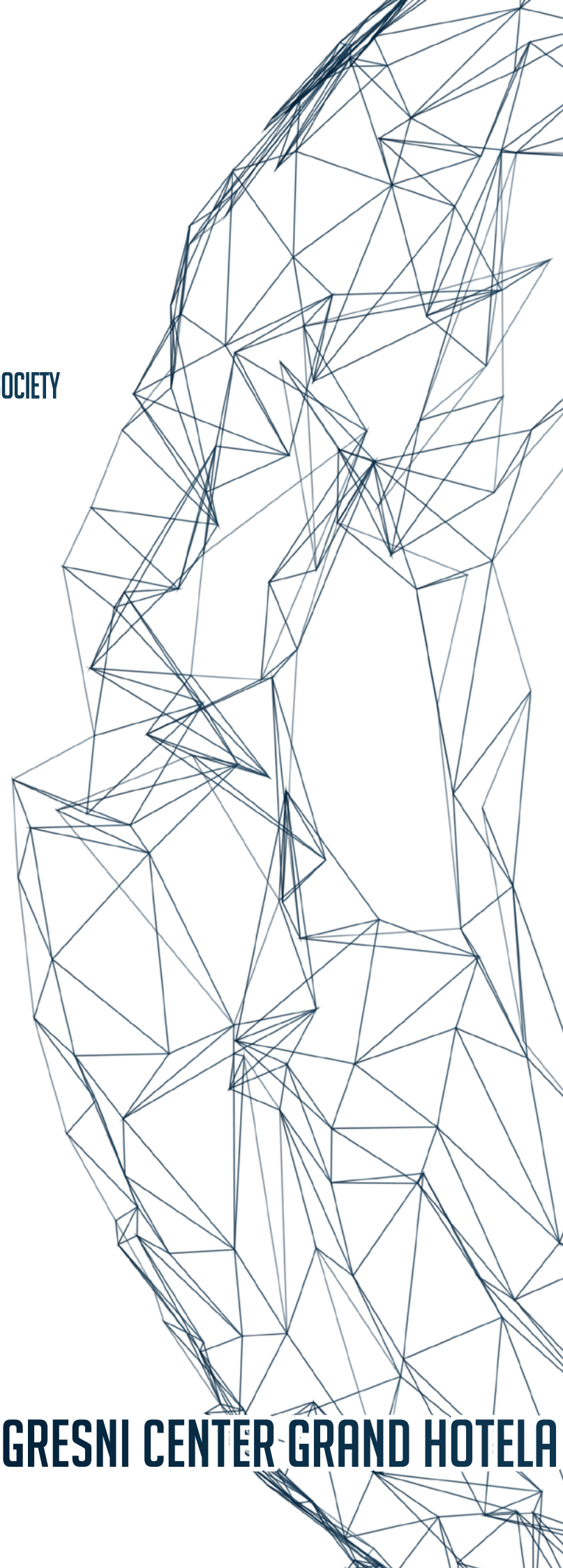

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NAGOVOR / PREFACE

BERNARDIN, PORTOROŽ

SPOŠTOVANE UDELEŽENKE, SPOŠTOVANI UDELEŽENCI KONFERENCE »SLOVENSKI KEMIJSKI DNEVI 2025«,

v imenu organizacijskega odbora in Slovenskega kemijskega društva vas prisrčno pozdravljam na 31. konferenci »Slovenski kemijski dnevi 2025«, ki bo potekala od 17. do 19. septembra v kongresnem centru Grand hotela Bernardin v Portorožu.

Tudi letos se bo konference udeležilo več kot 200 raziskovalcev in strokovnjakov iz Slovenije in tujine, med njimi številni predstavniki industrije. Dogodek ostaja odlična priložnost za mreženje, sodelovanje in izmenjavo izkušenj med kemiki in kemijskimi inženirji iz akademskega, raziskovalnega, industrijskega in upravnega okolja. Veseli nas, da bo med udeleženci tudi veliko doktorskih in magistrskih študentov, ki bodo s svojimi prispevki pomembno obogatili program. Za najboljše študentske prispevke in predstavitve, bodisi v obliki predavanj bodisi posterjev, bomo ob zaključku konference tradicionalno podelili diplome in denarne nagrade, ki jih letos omogoča podjetje Vigor iz Nemčije.

Na konferenci bo predstavljenih več kot 170 znanstvenih in strokovnih prispevkov v obliki plenarnih, vabljenih in sekcijskih predavanj ter posterjev, s poudarkom na področjih materialov, organske kemije, kemijskega inženirstva ter izobraževanja v kemiji. Med plenarne predavatelje smo povabili prof. dr. Joke Hadermann (University of Antwerp, Belgija), prof. dr. Güntherja Rupprechterja (TU Wien, Avstrija) in prof. dr. Silvio Gross (University of Padova, Italija). Kot vabljeni (keynote) predavatelji bodo sodelovali tudi dr. Matej Huš, prof. dr. Elena Bykova, dr. Martin Ocepek, izr. prof. dr. Gabriela Kalčikova, dr. Miha Drev, dr. Silvo Zupančič in prof. dr. Ewa Szczurek.

V času konference bo potekala tudi tradicionalna razstava laboratorijske, procesne in programske opreme ter literature, na kateri bo sodelovalo dvajset razstavljalcev.

Posebej bi želel izpostaviti delavnico »Veščine predstavitev na konferencah in komuniciranje znanosti: Govorite, da boste slišani«, ki je namenjena študentom, mladim raziskovalcem in raziskovalcem na začetku kariere. Delavnica, izvedena v okviru konference SKD 2025, bo udeležencem pomagala okrepiti samozavest pri javnem nastopanju, pridobiti praktične nasvete za pripravo in strukturiranje predavanj ter izboljšati veščine učinkovitega komuniciranja znanstvenih vsebin.

V četrtek, 18. septembra 2025, ob 20. uri ste lepo vabljeni na svečano slovesnost, na kateri bodo podeljene nagrade Slovenskega kemijskega društva.

Iskreno se zahvaljujem diamantnemu partnerju Vigor Gas Purification Technologies (Europe), zlatemu partnerju Lek d.d. ter vsem srebrnim in bronastim sponzorjem za podporo pri izvedbi konference. Ob tej priložnosti se zahvaljujem članom organizacijskega odbora za zavzeto delo pri oblikovanju programa ter izboru plenarnih in vabljenih predavateljev.

Želim vam uspešne predstavitve vašega dela, veliko zanimivih razprav in prijetno druženje v Portorožu.

S spoštovanjem,

znan. svet. dr. Albin Pintar
predsednik organizacijskega odbora konference

DEAR PARTICIPANTS OF THE 31ST ANNUAL MEETING OF THE SLOVENIAN CHEMICAL SOCIETY,

On behalf of the Organizing Committee and the Slovenian Chemical Society, it is my pleasure to welcome you to the 31st Annual Meeting of the Slovenian Chemical Society, which will take place from 17 to 19 September 2025 at the Grand Hotel Bernardin Convention Center in Portorož.

This year's conference will once again bring together more than 200 researchers and experts from Slovenia and abroad, including many representatives from industry. The event continues to be an excellent opportunity for networking, co-operation and exchange of experience between chemists and chemical engineers from the academic, research, industrial and administrative sectors. We are particularly pleased that many PhD and Master's students will participate and significantly enrich the programme with their contributions. As is tradition, the best student contributions and presentations, either in the form of papers or posters, will be honoured with certificates and cash prizes at the end of the conference, which is made possible this year by the support of the company Vigor from Germany.

More than 170 scientific and technical contributions will be presented at the conference in the form of plenary lectures, invited lectures, sectional lectures and posters, with a focus on materials, organic chemistry, chemical engineering and chemical education. We are honoured to have plenary lectures by Prof. Dr. Joke Hadermann (University of Antwerp, Belgium), Prof. Dr. Günther Rupprechter (TU Wien, Austria) and Prof. Dr. Silvia Gross (University of Padova, Italy). The keynote speakers also include Dr. Matej Huš, Prof. Dr. Elena Bykova, Dr. Martin Ocepek, Assoc. Prof. Dr. Gabriela Kalčikova, Dr. Miha Drev, Dr. Silvo Zupančič and Prof. Dr. Ewa Szczurek.

During the conference, there will also be a traditional exhibition of laboratory, process and software equipment and literature, in which twenty exhibitors will participate.

I would particularly like to emphasize the workshop "Conference presentation skills and science communication: Speak to be heard"," which is aimed at students, young researchers and early career scientists. This workshop, organized as part of the conference, will help participants to boost their confidence in public speaking, gain practical advice on preparing and structuring their presentations and improve their ability to communicate scientific content effectively.

You are cordially invited to attend the ceremony on Thursday, 18 September 2025, at 20:00, where the Slovenian Chemical Society awards will be presented.

I would like to thank our diamond partner Vigor Gas Purification Technologies (Europe), our gold partner Lek d.d. and all silver and bronze sponsors for their support in making this conference possible. I would also like to thank the members of the Organizing Committee for their dedicated work in designing the programme and selecting the plenary and keynote speakers.

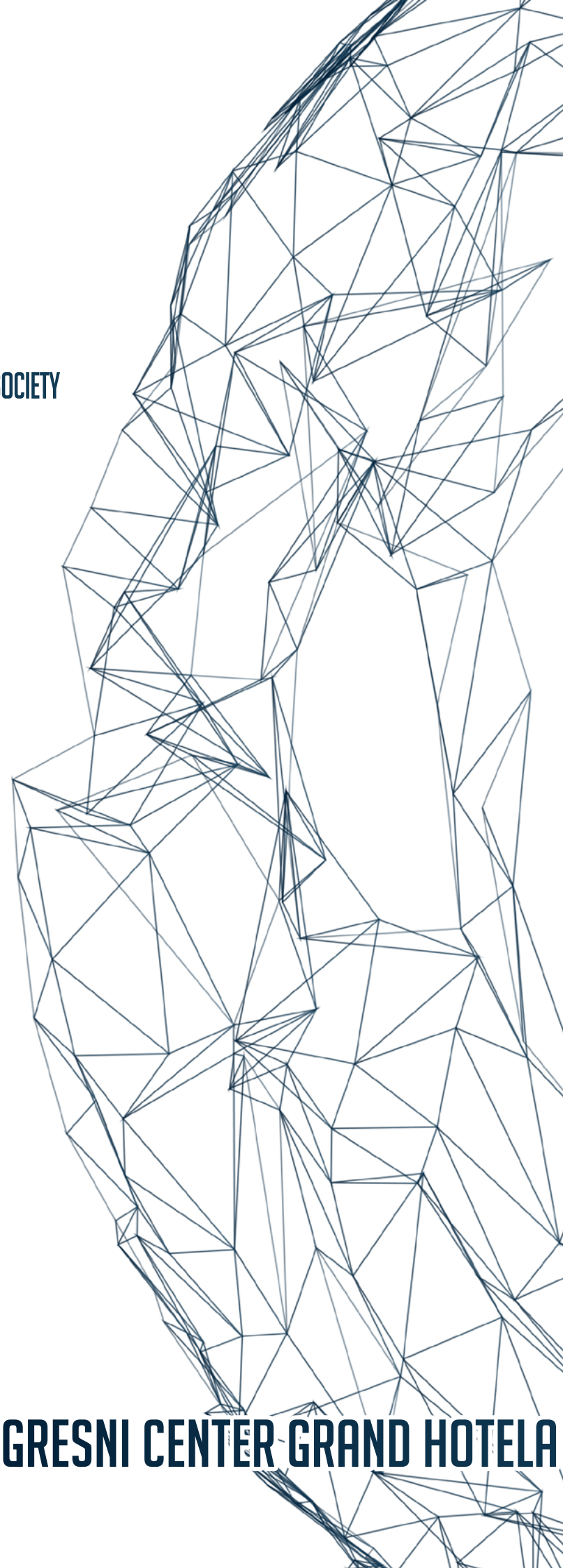
I wish you successful presentations of your work, many stimulating discussions and an enjoyable time in Portorož.

With kind regards,

Res. Prof. Dr. Albin Pintar
Chairman of the Organizing Committee

SLOVENSKI KEMIJSKI DNEVI 2025

31ST ANNUAL MEETING OF THE SLOVENIAN CHEMICAL SOCIETY



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PLENARY LECTURES

BERNARDIN, PORTOROŽ

Crystal structure evolution tracking using in situ 3D ED, in situ SNBD and 5D ED

Matthias Quintelier[a], Daphne Vandemeulebroucke[a], Maria Batuk[a], Amirhossein Hazijadeh[a], Sepideh Rahimisheikh[a], Saleh Gholam[a], Joke Hadermann[a]

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In situ diffraction is a powerful method for capturing diffraction patterns under dynamic conditions—such as changes in time, temperature, or pressure—while the sample remains in place. This enables the direct determination of crystal structures as they evolve. In the field of energy materials, in situ diffraction techniques have proven especially valuable: in situ neutron and X-ray diffraction have elucidated phase transformations in hydrogen storage systems, batteries, and oxygen ion conductors, as well as structural evolution during synthesis and crystal growth. However, such studies are often limited to powder diffraction, which collects signals from thousands of particles simultaneously and yields one-dimensional intensity-versus-angle profiles. These are frequently affected by peak overlap and broadening, complicating reliable structure solution. In principle, in situ single-crystal X-ray or neutron diffraction could overcome this, but it requires crystals several microns to millimeters in size—sizes that are often incompatible with relevant reactions due to, for example, prohibitively long ion diffusion paths.

Over the past decade, the advent of 3D electron diffraction (3D ED) has enabled structure solution and refinement from nanosized crystals. This opens the door to in situ single-crystal diffraction experiments on individual nanoparticles within polycrystalline powders. When combined with scanning approaches such as scanning nanobeam electron diffraction (SNBD), it turns into 5D ED, and it becomes possible to determine the crystal structures of many nanoscale crystals simultaneously, enhancing both statistical significance and representativity.

This lecture will explore the potential and challenges of in situ 3D ED and in situ SNBD, illustrated with examples involving redox reactions in batteries [1] and solid oxide fuel cells [2], gas incorporation and activation in metal-organic frameworks (MOFs) [3], and molecular (de)intercalation in layered double hydroxides (LDHs) [4], and will elaborate on the potential of 5D ED.

Keywords: in situ, 3D ED, SNBD, 5D ED

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From Applied Catalysis to Watching Chemical Surface Reactions on Single Nanocrystals

Günther Rupprechter

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In the transition from fossil to renewable resources, heterogenous catalysis remains a key technology in providing chemicals, fuels, energy and a clean environment. Significant advances often follow breakthroughs in fundamental understanding or the development of new concepts [1]. Along these lines, I discuss three recent case studies:

(i) To master contemporary challenges and reduce environmental impact, transforming hazardous and difficult-to-process waste will become crucial. We have converted spent Ni-MH batteries and aluminium waste into Ni/η-Al_2O_3 nanocatalysts for CO_2 hydrogenation with CH_4 selectivity of 99.8%. The mechanism was investigated by operando DRIFTS/GC+MS. To complete the upcycling/recycling loop, the spent Ni/η-Al_2O_3 was recycled into Ni and Al precursors [2].

(ii) Well-defined Ag nanoparticles, prepared by spark ablation and supported on graphite (HOPG), were characterized by various surface spectroscopy methods and electron microscopy. Employing an atmospheric pressure flow microreactor, the turnover frequencies (TOFs) of Ag/HOPG in ethylene hydrogenation up to 200 °C were found 200-times larger than that of unsupported Ag foil. DFT calculations indicated that H_2 adsorption was weak on unsupported Ag, whereas it increased by 0.5 eV for Ag/HOPG, driven by changes in Ag-Ag distances near the metal-carbon three phase boundary. H_2/D_2 scrambling corroborated a facilitated hydrogen activation at the metal-carbon interface, explaining its unique properties [3].

(iii) To directly "watch" a catalytic reaction on a metal nanoparticle, correlative surface microscopy was used: several techniques were applied under identical reaction conditions to the same metal nanotip (~30 nm), mimicking a single faceted nanocrystal. Field emission microscopy (FEM) and field ion microscopy (FIM) were employed for real-time *in situ* imaging of *facet-resolved* H_2 oxidation on a Rh nanocrystal, with and without La atom modifiers. This visualized not only the catalyst surface, but particularly the adsorbed reactants, so that active and inactive states could be discerned (kinetics by imaging), active regions identified, the effect of La adatoms revealed, and mechanisms elucidated [4].

Keywords: metal-carbon interfaces; ethylene hydrogenation; single particle catalysis; hydrogen oxidation; methanation

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The inorganic chemistry playground: optimising inorganic materials for a clean environment by navigating the experimental parameters space

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Clean environment and sustainable energy conversion and storage are presently among the most pressing issues to be addressed for a smooth energy transition in a circular economy framework. A careful materials selection and the optimisation of efficient, low-cost and environmentally friendly advanced inorganic materials for environmental protection, energy conversion and storage and catalysis are paramount. In a sustainable zero-emission and critical raw materials perspective, inorganic materials for these applications should however comply not only with the paradigms of green chemistry, as well as with these of its more recent implementation, circular chemistry, but also with further synthetic requirements. Low temperature of processing, use of benign and not hazardous and earth abundant precursors, use of water or not toxic/not flammable solvents, high yields, low energy and materials consumption, easy implementation at industrial scale, reprodicibility are only some of the basic requirements to be met. In this context inorganic materials chemistry represents an exciting playground for the design and optimisation of sustainable routes, and the resort to unconventional synthesis conditions discloses exciting perspectives in orienting, *inter alia*, the size, the morphology and the final structure of the crystalline materials. A valuable support can derive from the application of statistical or theoretical tools, enabling to rationalise the synthetic path and to minimise the experimental effort and the related energy and materials consumption. In this framework, in our group at University of Padua we have explored different low (T< 150°C) temperature and sustainable wet chemistry and colloidal routes to produce size- and shape-controlled inorganic nanomaterials for heterogeneous catalysis, gas exhaust abatement, energy storage. By exploiting unconventional experimental conditions disclosed by the different methods, i.e. not standard temperature and pressure or the confined space inside the miniemulsion-generated droplets, we prepared ferrites [1], manganites [2], pure and doped metal oxides, sulphides, halogenides, metal/metal oxide nanocomposites, supported metal nanoparticles and, recently, high entropy spinel oxides. The adopted wet chemistry routes ranged from i. miniemulsions [3] to ii. hydrothermal route to iii. microfluidic [4] and iv. classical colloidal routes [5-6]. Exciting results could be achieved by the combination of the above-mentioned routes [7] and by a systematic exploration of the broad parameters landscape, also supported by Design of Experiments [8].

Keywords: miniemulsion, hydrothermal, microfluidic, wet-chemistry, catalysis

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KEYNOTE TALKS

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Exploring chemistry at high pressures by means of single-crystal X-ray diffraction

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Many scientific disciplines, including chemistry, physics, materials science, and mineralogy, are interested in studying compounds under extreme conditions such as high pressures and high temperatures (HPHT). External stimuli can induce structural, electronic, and magnetic changes in matter; chemical reactions conducted at HPHT can exhibit unexpected behavior, entirely different from that observed under ambient conditions. However, analyzing and interpreting data collected at multimegabar pressures, especially during or after chemical reactions, is extremely challenging due to the often unknown and exotic chemistry of materials under these conditions.

Single-crystal X-ray diffraction in diamond anvil cells offers a unique opportunity to study, in situ, key characteristics of materials, such as their crystal structure (including unit cell parameters, space group, atomic coordinates, and atomic occupancies) and, when needed, phase composition. Here, we demonstrate the powerful capabilities and new opportunities that high-pressure crystallography offers to chemistry and materials science, using examples from studies of metal borides, iron oxides, and carbonates.

Keywords: single-crystal X-ray diffraction, diamond anvil cells, high pressures, iron oxides

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Chemistry in the Service of Life: A Comprehensive Approach to the Synthesis of Irbesartan

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One of the most important ways in which chemistry directly serves life is through the development and synthesis of active pharmaceutical ingredients (APIs) used in medicinal products. APIs are biologically active molecules that are essential for every medicine. Their role is to influence physiological processes in the body through a precisely defined mechanism of action, thereby contributing to the treatment, alleviation, or prevention of disease.

For an API to become part of a medicinal product, it must meet a number of requirements. Among the most important are high purity, repeatability and robustness of the synthetic process, and compliance with numerous regulatory guidelines and standards, such as GMP (Good Manufacturing Practice) and ICH (International Council for Harmonisation of Technical Requirements for Pharmaceuticals) [1]. Increasingly, environmental responsibility is also being emphasized, with synthetic processes expected to follow the principles of green chemistry and sustainable development.

A practical example in which all these principles are clearly demonstrated is Krka's development of synthetic processes for irbesartan, an active ingredient used in medicines for the treatment of arterial hypertension. This case study outlines all key stages of the synthesis development – from the initial selection of the synthetic route and strategy design, preparation of a suitable crystalline form of the API, and addressing challenges related to patent-protected final forms, to the scale-up of the process from laboratory scale to pilot and finally industrial scale. Four distinct synthetic processes for irbesartan were developed [2], each with a clearly defined purpose or objective, and a new pharmaceutically acceptable and useful salt of irbesartan was discovered [3].

The development of such synthetic processes brings with it many of the challenges faced by the pharmaceutical industry: identifying non-infringing synthetic routes, protecting proprietary knowledge and innovative approaches, preparing the final crystalline form of the API, and optimizing chemical reactions to be safe, efficient, and economically viable at large scale.

An important aspect of developing synthetic processes for industrial use is the approach to laboratory work itself: failed experiments are not merely discarded, but treated as a valuable source of insight and learning. Successful experiments are further optimized and incorporated into reliable, efficient, and sustainable production processes. In this way, chemistry transcends the boundaries of research and becomes a tangible tool in the service of life – contributing to health, quality of life, and broader societal well-being.

Keywords: active pharmaceutical ingredient, synthetic process, green chemistry, irbesartan

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Whatever the weather, we research together: talking theory to experimentalists

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Heterogeneous catalysis is the primary method to produce industrially relevant chemicals. More than 90 % of chemical industry relies on catalysts to steer reactions towards the desired products and reduce the energy expenditure. While the notion of catalytic reactions has been known for more than a century, the 21st century has seen a significant change in how catalysts are discovered, improved and modified. Trial-and-error, empirical correlations and experimental screening campaigns have been supplemented by computational modelling, which is promising faster, cheaper and more thorough catalyst discovery and in-depth understanding of their performance.

Ab initio models are built purely on theoretical insights and, in ideal cases, do not need experimental data. In practice, empirical data are useful to obtain catalyst structures, most relevant intermediates and experimental measurements to benchmark theoretical models against. Nevertheless, *ab initio* models are increasingly used to supply information that experiments alone cannot offer. [1]

Experimentalists and theoreticians therefore often work together. In their interactions, misunderstandings and unrealistic expectations might arise from both sides. Elaborate experimental techniques yield information that is not always immediately transferrable into theoretical models. On the other hand, theoretical modelling regularly makes assumptions that are poorly tethered to reality. While it is rewarding to arrive at the same conclusions from both perspectives, this is seldom achieved without several rounds of discussions and consultations.

In this talk, we will walk through the most commonly used theoretical and modelling techniques in modern heterogeneous catalysis and emphasize how they interact with experiments. We will focus on what experimentalists can learn from theoretical models and which input the latter covet the most. Density functional theory (DFT) [2], ab initio molecular dynamics (MD), kinetic Monte Carlo (kMC) and mean-field microkinetics (MKM) [3] will be discussed with emphasis on how they differ and what results they can provide. Examples of good practice will be presented. Finally, we will look at emerging trends, such as artificial intelligence and machine learning, which pose new challenges as they require large amounts of high-quality experimental data.

Keywords: quantum chemistry, heterogeneous catalysis, DFT, multiscale modelling

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N-Nitroso Hydrochlorothiazide
Stability, Degradation, and Safety Concerns

Miha Drev[a], Rok Grahek[a], Borut Zupančič[a], Matej Ošlaj[a], Andrej Bastarda[a], Andrej Kocijan[a], Zdenko Časar[a,b]

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Hydrochlorothiazide (HCT), a widely used antihypertensive drug, has recently attracted attention due to the potential formation of *N*-nitroso-hydrochlorothiazide (NO-HCT), a nitrosamine impurity of toxicological concern [1–3]. This study investigates the stability and degradation pathways of NO-HCT under physiologically relevant aqueous conditions (pH 1–8), with the aim of elucidating its degradation mechanism and assessing its potential risk [1].

The results demonstrate that NO-HCT is highly unstable in aqueous media, particularly at neutral to basic pH (6–8), where it rapidly degrades into several products, including formaldehyde, thiatriazine, and 2-amino-4-chloro-5-sulfamoylbenzenesulfonic acid. At lower pH values (1–5), the degradation is slower and yields a different impurity profile, notably including the reformation of HCT and, at pH 1, the formation of a sulfonyldiazonium salt in approximately 3% yield [1].

A key finding is that the potentially mutagenic aryl diazonium salt, which could theoretically form via metabolic activation of NO-HCT, was not detected in any degradation pathway. Instead, the sulfonyldiazonium species observed is chemically distinct and rapidly hydrolyzes in aqueous media, suggesting low toxicological relevance. The study also confirms that aryl diazonium salt can only be synthesized under highly acidic and anhydrous conditions, which are not physiologically relevant [1].

Mechanistic studies using NMR and LC-MS, supported by isotopic labelling and kinetic modelling, propose a degradation pathway involving diazohydroxide intermediates and parallel reaction routes influenced by pH. The formation of nitrosyl cation under acidic conditions was experimentally confirmed via trapping experiments [1].

In conclusion, NO-HCT degrades through well-defined chemical pathways that do not involve the formation of high-risk mutagenic species under physiological conditions. These findings support the argument that NO-HCT should not be classified as a cohort of concern compound [1, 3].

Keywords: hydrochlorothiazide, N-nitrosamine, diazonium, degradation, reaction mechanism

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Sustainable organic resins in coatings industry and beyond

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In recent years, industrial resins and coatings development trends have been significantly influenced by the escalating awareness of sustainability, evolving legislation, and customer expectations.

Current (industrial) research is focused on exploring potential substitutes for fossil-based building blocks for polymer (resin) synthesis to re-shift back to sustainable coatings. 2,5-Furandicarboxylic acid (FDCA) and set of Itaconic acid esters seems to be the most promising. Still, these novel systems must not only have lower environmental impact but also needs to meet all visual, protective, and other functional properties.

Recent published research on polyester- and acrylic- basis will be presented and critically evaluated from industrial feasibility [1-5]. Additionally, current research activities on the field and beyond will be presented.

Keywords: Resins, Coatings, Polyester, Acrylic, Itaconate

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Generative AI for Antimicrobial Peptide Discovery

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Generative AI emerged as a promising technique to revolutionize molecule discovery, in particular antimicrobial peptides [1,2]. The key challenge for applications of generative AI for molecule design is to equip the methods with controllability mechanisms, an area our lab has been recently actively contributing to. I will first describe two approaches for AI-driven antimicrobial peptide design, namely a conditional variational autoencoder-based model, called HydrAMP, and a controlled diffusion model OmegAMP. HydrAMP learns lower-dimensional, continuous representation of peptides and captures their antimicrobial properties [3]. The model disentangles the learnt representation of a peptide from its antimicrobial conditions and leverages parameter-controlled creativity. HydrAMP was directly optimized for unconstrained and analogue generation and outperforms other approaches in these tasks. Wet-lab validation experiments on five bacterial strains confirmed high activity of nine peptides generated by HydrAMP as analogues of clinically relevant prototypes, as well as six analogues of an inactive peptide. OmegAMP, offers a higher controllability than HydrAMP and is a framework that leverages a diffusion-based generative model with efficient low-dimensional embeddings, precise controllability mechanisms, and novel classifiers with drastically reduced false positive rates for candidate filtering [4]. OmegAMP enables the targeted generation of AMPs with specific physicochemical properties, activity profiles, and species-specific effectiveness. Moreover, it maximizes sample diversity while ensuring faithfulness to the underlying data distribution during generation. We demonstrate that OmegAMP achieves state-of-the-art performance across all stages of the AMP discovery pipeline, and leads to unprecedently high success rates in experimental validation, significantly advancing the potential of computational frameworks in combating antimicrobial resistance. I will also introduce our transformer-based model, Hyformer, which successfully blends the generative and predictive functionalities by using an alternating attention mechanism and a joint pre-training scheme. We show that Hyformer exhibits synergistic benefits in conditional sampling, out-of-distribution property prediction and representation learning. In application to antimicrobial peptide design, Hyformer obtained success rates comparable to OmegAMP and is now further applied to more challenging tasks. The talk will be closed by summarizing promises and challenges that remain to be addressed in the field.

Keywords: Generative AI, discriminative models, antimicrobial peptides

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Interactions of microplastics in the aquatic environment

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Plastic pollution is a pervasive and growing environmental problem, with microplastics becoming one of the biggest areas of concern. Once released into the aquatic environment, microplastics do not remain inert but undergo complex physical, chemical and biological transformations [1]. One of the most significant processes affecting microplastics in the aquatic environment is the formation of biofilm, which involves the colonisation of their surfaces by microorganisms. This biological aging process alters the physico-chemical properties of microplastics, including surface morphology and chemistry [2]. As a result of these changes, microplastics interact differently with their environment than their pristine counterparts. An important impact on the environment is their enhanced ability to adsorb and transport metals and other pollutants, which can lead to a localised increase in pollutant concentrations [3]. In addition, biofilms can serve as vehicles for the dispersal of microorganisms, including invasive or pathogenic species, allowing them to drift through ecosystems attached to microplastic surfaces [4]. In sediments, the presence of microplastics has been associated with altered biogeochemical processes, including increased production of greenhouse gases [5]. These effects emphasise the multifaceted and evolving role of microplastics as an active environmental agent rather than just a passive pollutant.

Given their widespread distribution and complex interactions in ecosystems, microplastics already have a measurable and significant impact on the environment. A comprehensive understanding of their transformation, ecological role and long-term impacts is essential to assess environmental risks and develop mitigation strategies. Continued interdisciplinary research is critical to addressing the challenges posed by microplastic pollution in the aquatic environment.

Keywords: effects, fate, plastic pollution, transformations, transport

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SLOVENSKI KEMIJSKI DNEVI 2025

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X-ray Absorption Spectroscopy for Structural Analysis of Amorphous Metal Oxide Thin Films

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Amorphous metal oxide thin films, such as aluminum oxide, nickel oxide, cobalt oxide, and iron oxides, serve diverse roles in catalysis and energy conversion. Al_2O_3 acts as a robust catalyst support due to its thermal stability, while transition metal oxides provide critical metal sites for catalytic reactions [1,2]. Understanding their atomic-scale structure (local coordination and oxidation states) is essential for optimizing performance. Amorphous metal oxide thin films, including Al_2O_3 supports and high-entropy alloy (HEA)-derived oxides, are engineered through thermal and electrochemical treatments to optimize atomic-scale structure. We employ X-ray absorption spectroscopy (XAS) to investigate how thermal densification governs Al^{3+} coordination in amorphous Al_2O_3 thin films, while a combination of thermal treatment and anodization transforms HEA surfaces into active electrocatalysts. Critically, surface-sensitive total electron yield (TEY) detection mode enables isolation of film-specific signals from substrates, allowing precise structural analysis.

For amorphous Al_2O_3, Al K-edge X-ray absorption near edge structure (XANES) and extended X-ray absorption fine structure (EXAFS) were measured on 300 nm films at different temperatures of thermal treatment (up to 1300 °C). XANES revealed a gradual coordination shift from tetrahedral AlO_4 (dominant below 400 °C) to octahedral AlO_6 (prevailing above 700 °C), driven by densification. EXAFS confirmed shortened Al-O bond distances above 700 °C, aligning with in-situ X-ray reflectivity data. Density functional theory (DFT) calculations using FDMNES on a model of amorphous alumina [3] reproduced the observed XANES spectral features, supporting the experimental interpretation of coordination evolution. Complementarily, a combination of thermal treatment and anodization of HEAs produces ~1 µm porous, catalytically active films. Using the surface-sensitive TEY detection mode (depth <100 nm), the catalytic layer was isolated from bulk substrates. XANES revealed HEA composition-dependent oxidation behavior: Fe was either fully oxidized to Fe^{3+} or remained metallic in Cr/Mn-rich alloys; Ni exhibited mixed Ni^{2+}/Ni^{3+} states; and Co converted predominantly to Co^{2+}. EXAFS confirmed the dissolution of metallic ordering and the appearance of nanostructured oxide-like local environments, linking the metal oxide layer to enhanced catalytic activity.

Surface-sensitive XAS provides critical atomic-scale insights into amorphous oxide thin films, enabling rational design of functional materials through precise structural characterization. We acknowledge the SOLEIL synchrotron facility (Paris, France) for the provision of beamtime for XAS experiments on the Lucia beamline (project 20230367) and Samba beamline (project 20240622).

Keywords: X-ray absorption spectroscopy, thin films, amorphous metal oxides

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High-pressure structural study of XeF_6

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The diamond anvil cell (DAC) is a device small enough to fit in one's hand (Fig. 1a), yet capable of generating pressures comparable to those found deep within the Earth's interior (>100 GPa). The DAC enables the investigation of chemical and structural changes under extreme conditions, granting access to materials and phases that may otherwise be unattainable, and that often exhibit exotic properties such as rare oxidation states, coordination numbers, or bonding modalities [1]. Among these are noble-gas compounds, but studies at high pressure remain rare and limited to theoretical predictions and commercially available samples due to the difficulties in their preparation and handling [2–4]. In this work, we present an experimental high-pressure study of XeF_6 [5]. Powder samples were loaded into DACs without a pressure transmitting medium inside a glovebox. Then, to induce recrystallization, samples were laser heated above 2000 K (Fig 1b), and structural changes were elucidated by synchrotron X-ray microdiffraction at the Extreme Conditions Beamline P02.2, PETRA III [6], and by Raman spectroscopy. The sample displayed rich polymorphism and an unprecedented hexameric unit, comprised of XeF_5^+ cations, F^- anions, and molecular XeF_6 with C_{3v}-like molecular geometry [7–9] experimentally observed for the first time.

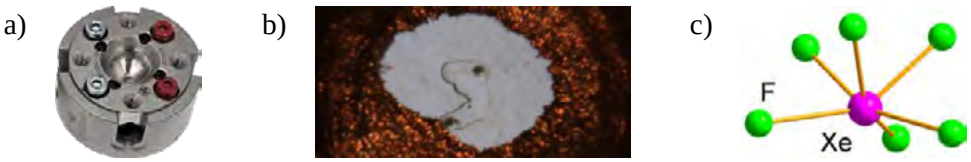

Figure 1. a) SS-DAC. b) Laser-heated sample in DAC. c) Structure of XeF_6 at 35 GPa with C_{3v}-like geometry.

Keywords: noble-gas compounds, high pressure, laser heating, single-crystal X-ray diffraction, synchrotron

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The influence of dispersing agents on micro-particle stabilization during film formation in sustainable industrial coatings

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In recent years, the industrial resins and coatings sectors have increasingly focused on the use of sustainable materials, in line with legislation and growing customer expectations [1]. As regulations become more restrictive, waterborne coatings have emerged as a logical choice for achieving more sustainable industrial coatings with lower volatile organic compound (VOC) content.

The incorporation and stabilization of microparticles in waterborne coating films is a critical step toward achieving stable colloidal systems and ensuring the desired protective end properties. However, the technical transition from solvent-based to waterborne systems requires a deep understanding of the associated challenges, particularly in terms of pigment wetting, foam control, long-term stability, and the ability to deliver high-performance final coating properties. While the use of surfactants plays a key role in this process, the experimental determination of optimal concentrations remains a significant challenge and impact on final coatings properties.

In this study, the stabilization of microparticles incorporated into waterborne (WB) coatings was investigated using surfactants, with quantification based on critical micelle concentration (CMC) titration measurements. Stabilisation behaviour of three different micro particles in the waterbased coatings were studied throught using electrochemical impedance spectroscopy (EIS) and rheology analysis. Several coatings formulations, varying in pigment volume concentration (PVC), were applied to standard steel substrates and monitored over a period of 30 days. Results demonstrate that EIS is a highly sensitive technique capable of detecting even minor deviations in surfactant concentration, which significantly influence the final anticorrosive performance of the coatings. Complementary rheological analysis further confirmed that the quantity of surfactant plays a critical role in the effective incorporation of microparticles within the colloidal coating matrix. At the end, the study highlights that optimal microparticle stabilization requires: precise determination of surfactant concentration via CMC analysis, and careful adjustment of PVC to enhance the barrier properties essential for long-term anticorrosive protection.

Keywords: Sustainable coating, surfactants, microparticle stabilisation, EIS

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Cardanol as a building block for UV hardening resins

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The potential of cardanol as a biobased molecule, which can be used as an interesting raw material for biobased UV curing resins, was the focus of the research. Commercially available biobased UV curing resins are usually based on oils and fatty acids, which do not offer the hardness needed for coatings. Therefore, those resins are mostly used as diluents to add the desired level of biobased component to the coating, as regulated by the authorities or the users. The potential of cardanol, with its aromatic ring, as a standalone biobased resin, which can be a true backbone of a coating, was identified. [1]

Cardanol is a phenolic lipid and is the main component of cashew nutshell liquid. Cashew nutshell liquid, a byproduct of cashew nut processing, makes it an interesting source of biobased chemicals that can be used for resins. It contains anacardic acid, cardol, and cardanol. Through thermal treatment of cashew nutshell liquid, the anacardic acid undergoes partial decarboxylation. With additional purification, cardanol is the result. The side chain on the meta spot of phenol varies in its degree of unsaturation. Tri-unsaturated cardanol is the major component, representing 40% of the mixture. On average, a molecule of cardanol has two unsaturated sites. The molecule is hydrophobic. [2]

The phenolic group, the active site of cardanol, can react with epichlorohydrin to add an oxirane ring to the molecule. Commercially available cardanol already reacted with epichlorohydrin was used during my research.

The double bonds on the side chain are the other useful reactive sites for the formation of oxirane rings. Epoxidation using the Prilezhaev reaction was used to produce additionally epoxidized cardanol. [3]

Described reactions formed an epoxidized cardanol with an average of three oxirane rings per molecule, which can be used as a surfactant for pigment wetting in coatings. The second step of the reaction was the acrylation step. The epoxidized cardanol was reacted with acrylic acid in the presence of a tin catalyst and inhibitors that prevented the polymerization of acrylic acid. At elevated temperatures close to reflux, the product was an acrylated molecule of cardanol with three sites with double bonds that can undergo polymerization. [4]

Synthesized resins were tested as reactive diluents and standalone resins in a UV curable formulation for wood coatings.

Keywords: cardanol, biobased, epoxidation, acrylation, UV hardening

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Chemical Substitutions and Single-Crystal Growth of $SrCu_2(BO_3)_2$

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The discovery of high-T_C superconductivity in doped cuprates in 1986 revealed chemical substitutions as a powerful route to accessing exotic ground states in frustrated, spin-gapped systems [1]. While one-dimensional (1D) spin-1/2 systems have been widely studied, two-dimensional (2D) analogues are scarce and less understood. A key 2D material is $SrCu_2(BO_3)_2$, where Cu^{2+} ions (S = 1/2) form orthogonal dimers within the *ab* plane, experimentally realizing the Shastry-Sutherland model [2]. Depending on the ratio of inter- to intra-dimer exchange interactions (J'/J), the system can host different ground states. With a $J'/J \approx 0.68$, $SrCu_2(BO_3)_2$ has the exact singlet-dimer ground state [3] and lies near a quantum critical point, providing a unique platform to explore the stability and evolution of a frustrated quantum antiferromagnet. Hydrostatic pressure has been shown to tune the J'/J ratio and induce quantum phase transitions [4]. In contrast, the effects of chemical pressure on the ground state of $SrCu_2(BO_3)_2$ remain less understood, mainly due to the difficulties in chemically modifying this compound. However, theoretical studies predict that chemical substitutions could tune the ground state, potentially leading to exotic magnetic phases such as quantum spin liquids or superconductors.

We explored the effect of chemical substitutions on the ground state of $SrCu_2(BO_3)_2$. Sr substitution by La achieved only up to ~2.6 mol% in single crystals, resulted in a clear reduction of the spin gap. Na substitutions, though very limited, only subtly increased the gap but introduced Cu hyperfine interactions in electron paramagnetic resonance spectra. Cu substitution by Mg led to a pronounced reduction of the spin gap, suppression of the pseudo-1/8 plateau, and the emergence of an anomaly at the onset critical field $\mu_0 H'_{C0} \approx 9$ T for ~7 mol% Mg [5]. Preliminary studies with Ni and Zn showed a subtle suppression of the spin gap. These findings confirm that, although partial, these substitutions still altered the magnetic interactions in $SrCu_2(BO_3)_2$. Current efforts focus on enhancing dopant incorporation via new synthesis strategies.

Keywords: chemical substitutions, 2D spin systems, magnetic frustration, spin gap, single-crystal growth

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Formaldehyde Emissions from Walls, Furniture, and Toys in Kindergartens: A Field and Laboratory Investigation

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Formaldehyde (HCHO) is a volatile organic compound (VOC) widely present in indoor environments, with documented adverse health effects ranging from mucosal irritation to carcinogenicity. This study aimed to quantify formaldehyde emissions from walls, furniture, and children's toys in Slovenian kindergartens, identify key influencing factors, and evaluate potential exposure risks for young children. Sampling was conducted in 22 kindergarten playrooms and one classroom, using passive samplers (filter paper and cotton) deployed for 7 days. Simultaneously, environmental parameters (room size, ventilation frequency, furniture age) were recorded via questionnaires. In addition, toys of varying materials and ages were analyzed for formaldehyde content. Laboratory analysis involved derivatization with pentane-2,4-dione and spectrophotometric detection at 436 nm, with calibration curves prepared from standardized formaldehyde solutions. Results indicated formaldehyde concentrations in indoor air ranging between ~14 ppb and 68 ppb, with higher levels associated with older buildings and less frequent ventilation. Toys made of painted wood and older textile toys exhibited higher formaldehyde release (up to ~71 ppb) compared to newer or polymer-based toys. These findings highlight the importance of building maintenance, adequate ventilation, and material choice in minimizing children's exposure to formaldehyde in educational settings. Our study aligns with previous findings showing that indoor formaldehyde concentrations are influenced by building materials, age, and ventilation patterns [1].

Keywords: Formaldehyde, Indoor air quality, Kindergartens, Volatile organic compounds, Passive sampling

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Environmental Chemistry in Slovenian Secondary School Textbooks: A Content Analysis for Sustainable Education

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Sustainable development is a central theme in today's education, which includes the promotion of scientific literacy and awareness of environmental challenges. Environmental chemistry plays an important role in promoting sustainable thinking among students [1]. Textbooks are still one of the most important sources of knowledge [2]; however, the extent to which they reflect current environmental issues is still unclear.

This qualitative study analyses the representation of environmental chemistry content in Slovenian secondary school chemistry textbooks approved for the school year 2024/2025. The main objective was to identify which environmental topics are included, how frequently they appear, and in what form they are presented. The methodological approach was based on the content analysis of textbooks, whereby the environmental topics were categorised into three key spheres: atmosphere, hydrosphere, and pedosphere.

A total of 19 textbooks were evaluated using two sets of criteria: (1) organisational-technical (general) and (2) content-didactic (textual and visual) [3]. The results show that certain topics — such as greenhouse gases and stratospheric ozone depletion — are well addressed, others (e.g. pesticides, pharmaceutical residues and microplastics) are barely mentioned or not mentioned at all. The analysis also reveals considerable deficits in the visualisation of content: Many textbooks lack multimedia or visual elements that could support the understanding of complex environmental processes.

The study concludes that a meaningful revision of textbooks is necessary, focussing on the integration of current environmental topics and improved visual support. In addition, it is recommended that teachers be encouraged to use textbooks more frequently and in a more targeted way in chemistry lessons.

Keywords: environmental chemistry, upper secondary school chemistry textbooks, textbook analysis

Acknowledgement

The authors acknowledge the financial support from the Slovenian Research and Innovation Agency through research core funding “Strategies for Education for Sustainable Development applying Innovative Student-Centered Educational Approaches” (ID: P5-0451).

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Izvedba šolskih kemijskih poskusov preučevanja oljčnih olj Slovenskega primorja vključno z metodami termične analize

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Kemijska obravnava lokalno obarvane tematike, oljkarstvom, kot eno izmed pomembnejših gospodarskih dejavnosti Slovenskega primorja, je lep primer ozaveščanja dijakov k poglobljenemu razumevanju problemov dejavnosti, ohranjanju tradicije in povezovanja z lokalno skupnostjo, tako pridelovalci kot raziskovalci.

Kemijska sestava oljčnih olj in s tem lastnosti olj, je odvisna od različnih dejavnikov. Nanjo lahko vpliva vrsta oljk, ki so bile uporabljene za pripravo olja, čas, ko so bile oljke pobrane in mnogo drugih dejavnikov.

Pri preučevanju oljčnih olj lahko uporabimo metode termične analize, ki so sicer kompleksne in težje dostopne za uporabo v srednjih šolah, so pa že v široki uporabi v bližnji industriji ali raziskovalnih institucijah. Termično stabilnost lahko proučujemo med segrevanjem v različnih atmosferah na TGA instrumentu, čas inducirane oksidacije (OIT) pri določeni temperaturi lahko določimo z DSC meritvijo [1]. Časi OIT olja pri različnih temperaturah pa so preko Arrheniusove enačbe osnova za izračun aktivacijske energije (*E*a) za oksidativni razpad olj. Na osnovi predhodnih meritev bom prikazala primer reševanja teoretične naloge za nadarjene dijake.

Preprostejši za izvedbo in razumevanje v srednji šoli pa so eksperimenti za določevanje lastnosti olj. Stopnje nenasičenosti maščobnih kislin določimo kot jodovo število (IV), ki predstavlja maso joda v gramih, ki se veže na 100 g olja. Uporablja se Wijsov postopek po standardni metodi, ki jo priporoča AOAC [2] ali preprosteje z raztopino joda in kalijevega jodida [3]. Kislinsko število (KŠ) je definirano kot masa kalijevega hidroksida v miligramih, ki nevtralizira proste maščobne kisline v 1 g olja. Podoben pomen ima kislost, ki jo izrazimo v % vsebovane proste oleinske kisline [2]. Kvalitativno pa lahko dokažemo prisotnost antioksidantov z nastankom temno modre oborine, imenovane železov(III) heksacianidoferat(II) ali prusko modra.

Nekatere eksperimente smo preizkusili kot demonstracijsko laboratorijsko vajo s kratkim teoretičnim uvodom v dveh oddelkih 3. letnika Gimnazije Koper. V teoretičnem uvodu sem dijakom najprej razložila sestavo oljčnih olj, predstavila oba eksperimenta, ki smo jih izvedli in na kakšen princip delujeta. Laboratorijska vaja je bila sestavljena iz dveh delov, določanja stopnje nenasičenosti z raztopino joda ter določanja kislinskega števila in kislosti. Po končani vaji so dijaki anonimno odgovorili na anketo. Večini dijakov je bila vaja zanimiva in poučna.

Tematika omogoča tudi razširitev v naravoslovni dan kot primer medpredmetne povezave z obiskom pridelovalcev oljk, oljarne ter lokalno prilagoditev tematike na preučevanje drugih olj, kot je bučno, sončnično...

Ključne besede: oljčno olje, termična analiza, šolski eksperimenti za gimnazije

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Motivation and Perceived Giftedness in Learning the Chemistry Triplet: A Study with Pre-Service Primary School Teachers

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Learning chemistry requires an understanding of its triple representational nature – the macroscopic, submicroscopic and symbolic levels – which can have a significant impact on student motivation. Difficulties in linking these levels can hinder conceptual understanding and lead to lower engagement in learning chemistry [1,2]. According to self-determination theory SDT, motivation is enhanced when students experience autonomy, competence and relatedness. In chemistry education, this theory helps to explain how students' perceived competence can decrease when they are confronted with abstract and complex content [3]. Gifted students need learning environments that support intrinsic motivation and promote autonomy through intellectually challenging tasks [4]. This project builds on the integration of SDT and the triplet model to investigate the motivational factors that influence gifted students' learning in chemistry and to support their development through conceptually coherent and inquiry-oriented instruction.

The purpose of the research is to determine pre-service primary school teachers' level of motivation for learning chemistry, level of intrinsic motivation for learning the chemistry triplet and the level of self-perceived giftedness for chemistry. The aim was also to find out whether there are correlations between these variables. 80 first-year preservice primary school teachers from the University of Ljubljana, Faculty of Education took, part in this quantitative study. Three questionnaires were used to collect data: a) motivation for learning chemistry [3], b) intrinsic motivation for learning the chemistry triplet [2], c) self-perceived giftedness in chemistry [4].

The comparative analysis using the Kruskal-Wallis test revealed statistically significant differences in students' motivation for learning chemistry across groups with different levels of intrinsic motivation for learning the chemistry triplet. Significant differences were found at the macroscopic level ($\chi^2(2, n = 80) = 17.633, p < .001$), the submicroscopic level ($\chi^2(2, n = 80) = 21.742, p < .001$) and the symbolic level ($\chi^2(2, n = 80) = 11.059, p = .004$). The students' motivation to learn chemistry also differed significantly across groups with different levels of perceived giftedness ($\chi^2(2, n = 80) = 10.202, p = .006$). In addition, significant differences were found between perceived giftedness and intrinsic motivation for learning each level of the chemistry triplet; macroscopic ($\chi^2(2, n = 80) = 15.910, p < .001$), submicroscopic ($\chi^2(2, n = 80) = 9.285, p = .011$), and symbolic ($\chi^2(2, n = 80) = 12.324, p = .002$) levels.

These findings indicate that students' motivation to learn chemistry significantly influences their motivation across the different representational levels of the chemistry triplet. Furthermore, enhancing students' self-perception of their scientific aptitude may be particularly critical when they are engaging with complex and abstract content of the chemistry triplet.

Keywords: triple nature of chemical concepts; motivation for learning chemistry; self-determination theory; giftedness in chemistry

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Philately and Chemistry

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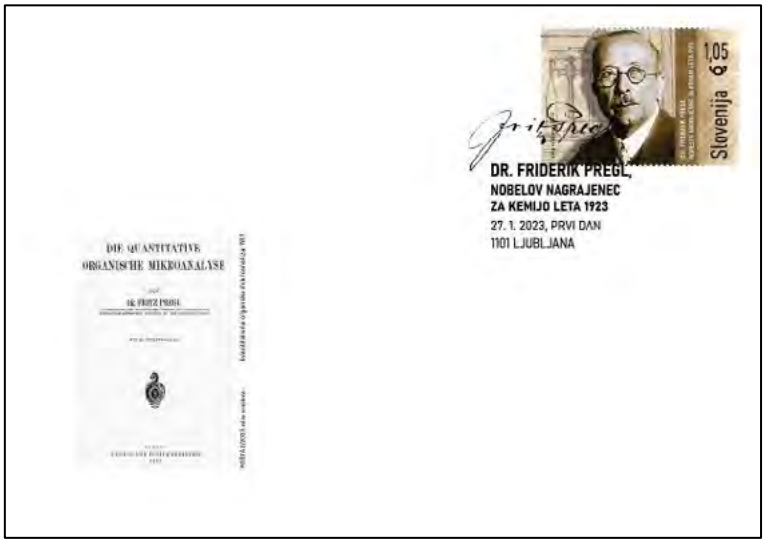
Stamps and other philatelic materials are issued to commemorate events and to educate the public. It is obvious that the rise of digital communication and online services have significantly reduced the need for physical mail and also stamp usage. Nevertheless, stamps are still in use and will undoubtedly continue to attract collectors also in the future. Chemical topics are not very often depicted on stamps but still many beautiful and interesting examples have been issued over the years in various countries of our planet [1-4].

In my lecture, I will briefly walk through the history of chemistry and some related subjects. I will start in the distant history and show how people started to deal with chemistry even though they did not yet know what chemistry is. I will also talk about the alchemists, introduce some of the pioneers of chemistry and some of the most distinguished chemists (A. Lavoisier, D. I. Mendeleev, M. Curie…). The Post of Slovenia has also issued some stamps related to chemistry, including a stamp dedicated to the Slovenian-born Nobel Prize winner Friderik Pregl (stamp and first day cover shown below) [5]. Some of the materials of this type will also be shown.



Keywords: chemistry; philately; stamps

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The development of primary school students' chemical literacy in non-formal educational environment

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The study explores the impact of the non-formal forensic module (NFFM) on the development of chemical literacy and selected motivational and cognitive factors among 8th-grade primary school students. It investigates the extent to which the module contributes to improvements in chemical literacy and which personal (e.g., motivation, self-concept, interest, formal-logical reasoning) and environmental factors (e.g., learning environment, collaborative learning) statistically significantly influence students' academic performance.
Based on a systematic literature review [1] following the *PRISMA* method, a learning module was designed and supported by the learning booklet *Chemical Detective*, which incorporates a forensic context that students can easily relate to. The module was implemented with 100 students from five primary schools. The study combined quantitative and qualitative methods aligned with the scientific research process from planning and instrument development to data collection, analysis, and interpretation. Data were collected through knowledge tests, questionnaires, observations, and semi-structured interviews. The results showed a statistically significant improvement in chemical literacy ($t(99) = -8.691$; $p < 0.001$; $d = 0.87$) and notable positive changes in student interest, motivation, and self-concept. Formal-logical reasoning ($R^2 = 0.298$) emerged as the strongest predictor of students' chemical literacy development, followed by self-concept ($R^2 = 0.237$) and motivation ($R^2 = 0.160$). Participants perceived the program as experimental, inquiry-based, and relevant to real life, which aligns with the findings on the effectiveness of context-based chemistry education [2, 3]. The program is built on components that actively engage students in the phases of scientific inquiry, such as hypothesis formulation, experimental planning and implementation, and data interpretation. The findings confirm the value of modern didactic approaches that incorporate context-based and inquiry-driven chemistry teaching. The *NFFM* program has proven to be an effective pedagogical model, whose core elements problem-based learning, collaborative activities, experimental work, and narrative framing are worth integrating into formal education. Such integration supports the development of chemical literacy and fosters students' interest and engagement in chemistry and the natural sciences [2, 3].

Keywords: chemistry, elementary school students, non-formal education, context-based chemistry learning, inquiry-based chemistry

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Measuring the heating efficiency of magnetically heated catalyst

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Induction heating catalysis, the use of an alternating magnetic field to apply heat directly to the catalyst has been a hot topic for over a decade [1]. The use of induction heating opens the possibility to build energy efficient, highly flexible and sustainable reactors.

One of the main issues in constructing an effective magnetically heated catalyst is predicting the heating properties of the magnetic nanoparticles. It has been shown earlier that the unusual kinetic effects observed for the inductively heated catalysts can be explained by assuming that the temperature of the nanoparticles is much higher than that of the reaction medium [2,3].

High-temperature calorimetric studies of various magnetic nanoparticles, including Co-Ni based catalysts for ammonia synthesis [4] were performed at the temperatures up to 600°C under controlled reducing atmosphere. A custom-made high-temperature differential calorimeter was constructed to study magnetically heated catalysts under induction heating.

The dependency of magnetic heating effect on temperature and magnetic field induction was obtained. A theoretical model of heat dissipation for highly inhomogeneous systems was provided. Based on this model the temperature of the magnetic nanoparticles was calculated and found to be higher than that of the surrounding medium.

The research was founded by European Union's Horizon Europe Research and Innovation Programme, under Grant Agreement n° 101177996.

Keywords: Induction heating; Magnetically heated catalyst; Calorimetry;

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Modulating Metal-Support Interactions: Ruthenium on MXene for CO_2 Hydrogenation

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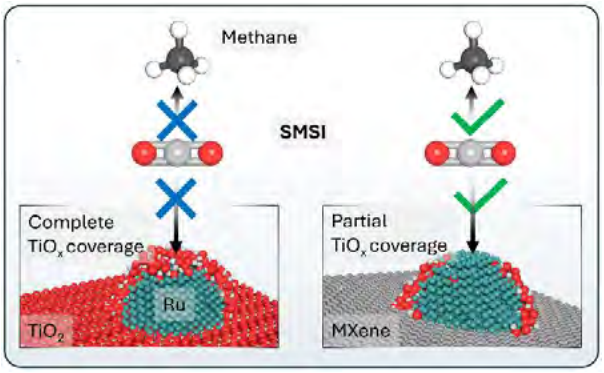

Controlling the selectivity of CO_2 hydrogenation to produce value-added fuels and chemicals is an actual challenge in catalysis research. Recently, a versatile class of two-dimensional transition metal carbides and nitrides (MXenes) has gained attention as a support in CO_2 hydrogenation, offering exceptional electron transfer capabilities and metal-support bonding [1]. However, while metal–support interactions have been extensively studied on various TiO_2 phases [2], their behavior on MXene remained unclear, particularly under conditions where surface oxidation may lead to TiO_2-like characteristics during extended operation.

In this study, we investigated RuO_2 nanoparticles supported on MXene or TiO_2 for CO_2 hydrogenation at atmospheric pressure. Although lower surface area and less uniform RuO_2 dispersion were observed on MXenes than on TiO_2, Ru/MXene exhibited superior catalytic activity, demonstrating that its unique textural properties and active site availability compensated the lower surface area. Higher Ru loading on MXene increased the methane selectivity and conversion, whereas lower loading favoured CO formation, highlighting the importance of optimizing catalyst loading. *Operando* DRIFTS analysis revealed the critical role of methoxy intermediates in affecting the catalytic pathway, suggesting potential for tuning synthesis conditions to improve yields. A partial encapsulation of Ru on MXene enhanced catalytic performance, while the strong metal support interaction (SMSI) effect on TiO_2 led to complete encapsulation, reducing catalytic efficiency. The environmentally conscious synthesis route, combined with detailed structural and spectroscopic characterization, offers a sustainable and tunable platform for designing future catalysts.

Keywords: ruthenium, MXene, TiO_2, SMSI, CO_2 hydrogenation

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Ammonia cracking for dynamically responsive H_2 release utilizing magnetically-heated catalyst

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Green hydrogen is emerging as a vital energy carrier. However, storing and transporting it in pressurized or liquid form remains both costly and hazardous [1]. Safer alternatives—such as storing hydrogen in molecules that can reversibly bond and release it on demand—are becoming increasingly important. One promising hydrogen carrier is ammonia. Yet, conventional ammonia decomposition reactors, which rely on thermal heating, face challenges such as delayed start-up due to limited heat transfer [2].

In this study, we report a method for the electrified, dynamically responsive decomposition of ammonia to release chemically bonded hydrogen on demand [3]. This is achieved through the rapid magnetic heating of a hierarchical nanocomposite catalyst. The catalyst comprises ferromagnetic CoNi alloy nanoparticles embedded in high-surface-area alumina, which is further decorated with catalytically active Ru nanoparticles.

The CoNi precursor nanoparticles were synthesized via a simple aqueous co-precipitation of Co^{2+} and Ni^{2+} ions using a basic solution. These were then embedded in alumina by hydrolyzing AlN in a colloidal suspension [4]. Subsequent reduction converted the CoNi precursors into a metallic alloy. Ru nanoparticles were deposited on the alumina surface through precipitation followed by reduction.

Experimental results, supported by density functional theory (DFT) calculations and microkinetic modeling, confirm a rapid, minute-scale response for hydrogen release. This fast activation suggests that the catalytic system could, in principle, enable the effective use of intermittent renewable electricity and provide a tunable H_2/NH_3 ratio in the reactor effluent.

Keywords: magnetic heating, catalysis, ammonia, hydrogen

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Biology as a Second Language: Functional Thinking for Structurally Trained Chemists

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Chemistry and biology often operate under fundamentally different conceptual frameworks. Chemists are trained to define and characterize molecular structure, while biological research typically begins with observed functions or phenotypes, without knowing the molecular players involved. As a result, a chemist's first question is typically *What is it?*, whereas a biologist tends to ask *What it does?* This divergence becomes particularly apparent in multidisciplinary collaborations, where effective communication and problem-solving demand a shift in perspective on both sides.

In this talk, I will reflect on these dynamics through my experience as a senior chemist in the MitoCan project, a collaborative effort to develop anticancer agents targeting mitochondrial ion channels. In early project meetings, the chemists presented synthetic route optimizations, late-stage diversification strategies, physicochemical profiles of lipophilic cations, counterion effects, and structure–activity relationships, only to find it was all "hexagons" to the biologists. Meanwhile, we were met with acronyms like JC-10, MTT, MTD, FCCP, and TMRM, and asked to choose among COLO-357, B16F10, C2C12 and NHLF cell lines: an avalanche of functional terminology that felt equally opaque.

A key breakthrough in learning to establish mutual language was simply to be more specific. Instead of "cytotoxicity," the chemists would say "reduction in viability as measured by resazurin assay in COLO-357 cells after 72 hours," while appreciating that even this could reflect reduced metabolism rather than cell death. Likewise, "compound ULEID-11" would be referred to by a biologist as "compound ULEID-11, batch 124-T3, stored in a plastic vial as a DMSO stock at room temperature since February." Understanding assay reagents at the structural level allowed the design of better bioactivity experiments as well as allowed us to recognize that "is the dye fixable?" really meant "does it react with formaldehyde," or that MitoTracker Deep Red is chemically closer to Green than to Red.

Once a common language was established, the project could fully benefit from the chemists' reductionist mindset and the biologists' systems-level tools.[1] This interdisciplinary synergy enabled the development and rigorous validation of novel mitochondria-targeting moieties with benchmark accumulation efficiency and minimized intrinsic bioactivity.

Keywords: chemistry, drug design, mitochondria

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Aggregate suppression of proteins by ATP analogs

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Biopharmaceutic proteins represent the fastest growing class of all pharmaceutical products. Challenges in their production and storage stem from their high molecular weight and structural complexity, as well as from instabilities that often lead to a loss of quality or efficacy due to formation of protein aggregates. Protein self-association and aggregation are thus considered major issues during production, often limiting the shelf-life of the product.(1,2) Protein aggregation occurs through association of so-called aggregation prone regions (APR), which are only transiently present in solution and hence experimentally difficult to detect and isolate. Current approaches to improve protein stability mostly focus on protecting the native structure of the biopharmaceutic proteins, often by adding excipients into final formulation. Adenosine triphosphate (ATP), a key cellular energy metabolite, has been shown to modulate protein self-assembly processes such as amyloid formation and the behaviour of biological condensates through non-specific, proteome-wide mechanisms and was identified as a potential stabilising additive for biologics (3,4). In each case, reduced ATP levels trigger widespread protein condensation and precipitation, while elevated ATP levels are required to promote disaggregation. The stabilizing properties of ATP can be attributed to its hydrotropic character, arising from its combination of a non-polar adenosine moiety and a highly charged triphosphate group through which ATP interacts with protein surface and stabilises it against aggregation. However, ATP spontaneously hydrolyses in water making it unsuitable for long-time storage of biologics.

To overcome this issue, we have designed a library of 48 compounds that exhibit a similar amphipathic property than ATP and evaluated their effects on aggregation of a model protein. Initially, we evaluated their effect on protein thermal and colloidal stability as well as assessed how they affect the kinetics of its aggregation. Using NMR we tested which excipients bind to the model protein, determined the strength of the interactions and evaluated whether the additive bind to the native or partially unfolded protein.

Keywords: biologicals, protein-protein interactions, NMR, additives

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Recent Progress in Thermochemical Energy Storage Materials

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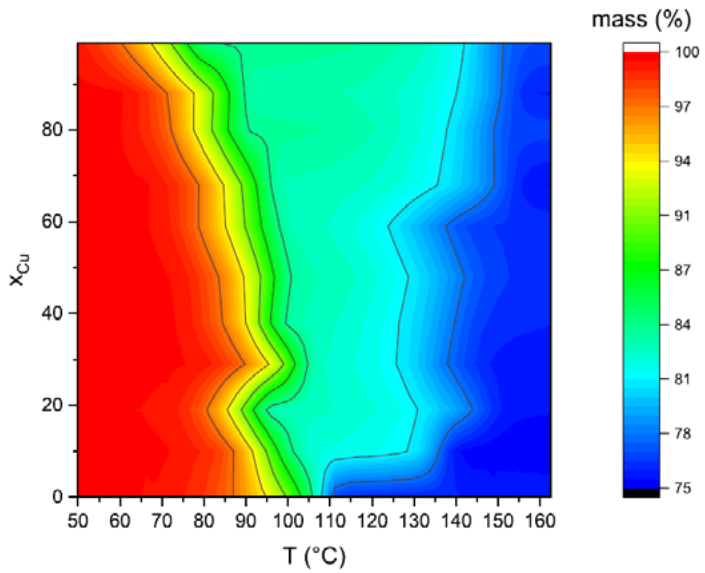
There are still plenty of challenges and obstacles for thermochemical energy storage materials (TCM) *in praxi* [1]. However, investigations of new salt hydrates showed recently a progress in tuning the material properties according to application needs, i.e. the operation temperatures. One promising class of materials are the Tutton Salts with a highly flexible range of molecular composition [2]. A thermogravimetric analysis of $K_2Zn_{1-x}Cu_x(SO_4)_2 \cdot 6H_2O$ shows an average first dehydration onset temperature of 81.5 °C (see Figure).



Upon variation of the molar composition of the bivalent cations Mg, Co, Ni or Cu with Zn four series of compounds were prepared and characterized, thus allowing for a tunable TCM according to application needs.

Furthermore, mixed sulfates of magnesium, cobalt, nickel, copper, and zinc have been investigated and their composition dependent properties elaborated [3]. Particle integrity and morphology is playing a key role in cycle stability. Single particle *in-situ* SEM observed dehydration process can yield insight into expected performance upon dehydration-rehydration cycles.

Keywords: thermochemical energy storage materials; salt hydrates

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Effect of surface chemistry on the saturation magnetization of barium hexaferrite nanoplatelets

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Barium hexaferrite nanoplatelets BHF NPLs are a special magnetic material that possesses uniaxial magnetocrystalline anisotropy combined with a shape anisotropy, resulting in thin hexagonal crystals with a magnetic easy axis perpendicular to the basal plane. BHF in the form of NPLs can be colloidally stabilized in various liquid media to form the only known room-temperature ferromagnetic liquids [1]. In addition to the above, surface chemistry was of equal importance for the development of the ferromagnetic liquids. In both systems [1], the surfactant dodecylbenzenesulfonic acid was used. However, during the development of new ferromagnetic systems [2], the NPLs' surface chemistry had to be tuned accordingly.

We investigated various surface ligands from the catechol and phosphonic-acid family and their adsorption on the surface of BHF NPLs, experimentally and theoretically. A stronger interaction of the phosphonic ligands was predicted with computational modelling and confirmed experimentally. However, a stable adsorption was obtained with some catechols, i.e., pyrocatechol and caffeic acid, under acidic conditions. Although not expected from the computations, the room temperature saturation magnetization of the BHF NPLs increased after phosphonic acids or catechols were robustly adsorbed on their surfaces. We investigated whether the observed increase is related to the mode of adsorption (e.g., chemisorption vs physisorption) or to the temperature effect on the magnetization. We compared the BHF NPLs functionalized with the selected ligands under different conditions and their saturation magnetization at room temperature and at 2 K. In the latter case, we can neglect the temperature effect on the magnetization and compare the measured magnetic properties with the calculated ones.

Keywords: barium hexaferrite, nanoplatelets, surface chemistry, adsorption, magnetization

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Acknowledgment. The authors acknowledge the financial support from the Slovenian Research and Innovation Agency through the research core funding P2-0089, and the projects N2-0367, P1-0192. The authors (T.L., M.C.) also acknowledge the project 24-10247K (the Czech Science Foundation).

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Hybrid SiO_2-Activated Carbon Monolithic Sorbents for Absorption-Peak Targeted Photothermal CO_2 Regeneration

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Carbon Capture, Utilisation and Storage (CCUS) technologies face major challenges, especially due to the high energy costs of the sorption–desorption cycle. While CO_2 capture is well-studied, the development of efficient and energy-effective desorption methods remains largely overlooked [1, 2].

An alternative way to reduce the energy of desorption process is to heat the sorbents locally, for example using light, i.e., photothermally triggered (PT) CO_2 desorption. Although sunlight is a sustainable energy source, its broad and fluctuating spectrum limits the efficiency of photothermal (PT) conversion, as PT materials typically exhibit narrow absorption peaks. Therefore, narrowband light sources, especially those with wavelength that match the material's absorption maximum (λ_{max}) are essential to maximize the PT conversion at given light power.

The first step toward energy efficient PT-driven CO_2 desorption is to develop thermally stable monolithic sorbents with long-term regeneration capability—something current amine-based solid and/or liquid systems struggle to achieve. Possible option to meet these requirements are porous, non-amine-based monolithic sorbents e.g., silica–activated carbon composites. Here, silica serves as the CO_2 sorbent and activated carbon primarily provides photothermal functionality, with added sorption capability.

Hybrid monoliths with various concentrations of incorporated loofah pumpkin-derived activated carbon fibres were prepared using a sol-gel templating method, followed by pyrolysis and activation [3]. The resulting hybrid monoliths exhibit hierarchical porosity, with pore sizes ranging from 0.5 nm to tens of microns. Their CO_2 sorption capacity depends on the activated carbon fibre loading, reaching the maximum value of 2 mmol/g at 0°C, outperforming pure silica monoliths for more than 50%. Thermally programmed desorption revealed that threshold temperature needed to desorb majority of captured CO_2 is ≈ 60° C, while for complete regeneration ≈110 °C is needed. The hybrid monoliths demonstrated excellent long-lasting cycling stability, whit only a 5% decrease in efficiency after 50 cycles. PT experiments were preformed using both, narrowband and broadband (solar-simulator) light sources at various powers. As expected, narrowband lights were more effecting. Already at the lowest power of 1 sun (≈ 0.1W) the threshold temperature needed for CO_2 desorption was reached within few seconds, while temperature for complete regeneration was achieved in ≈ 30 s. In contrast, with broadband light of same power, not even the threshold temperature was reached.

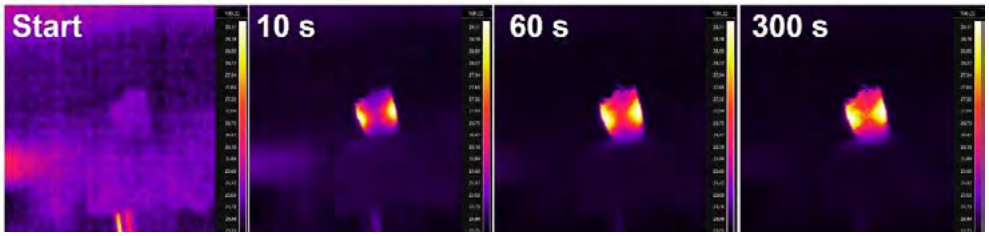

Figure 1: Thermographic images of silica–activated carbon hybrid monoliths heated under narrowband light

Keywords: carbon capture and utilization, photothermal effect, hybrid monoliths, sustainability

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Acknowledgments: Projects HELICOSS (N2-0389 and J2-6003) and programme P2-0412

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Simple and Fast Wettability Control of Aminosilanized Surfaces with Carboxylic Acids

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Reversible surface wettability is a key feature of smart coatings used in self-cleaning materials [1], microfluidics, anti-icing surfaces, and separation technologies [2]. Many existing approaches rely on stimuli-responsive materials such as photochromic azobenzenes, thermally activated oxides, or plasma-treated surfaces [3], but they typically require prolonged processing, complex synthesis or expensive instrumentation. In this work, we present a fast and fully reversible method for modulating surface hydrophobicity on glass using common carboxylic and mineral acids. The approach is based on the formation of ionic pairs between aminosilanized surfaces and acidic groups, enabling wettability switching within minutes using simple acid/base rinsing cycles.

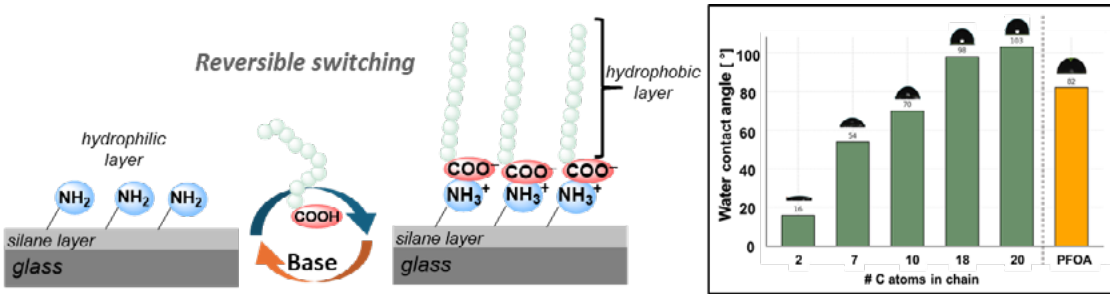

Figure 1: Left: Ionic pairs formation on the surface of aminosilanized glass substrate with long chain carboxylic acids that form a hydrophobic monolayer on the surface. Right: Water contact angle determination for aminosilanized substrates protonated with carboxylic acids with varying chain lengths.

We will describe the preparation and optimization of aminosilanized glass surfaces using oxidation pre-treatment and vapor-phase silanization. These surfaces allow controlled modulation of surface polarity through ion pairing with mineral or organic acids. The system's wettability can be predictably tuned by the acid's molecular structure, and the switching process is fully reversible. This simple approach eliminates the need for light, heat, or electronic input and provides a robust platform for next-generation surface coatings.

Keywords: Reversible wettability, aminosilane, carboxylic acid, ion pair, self-cleaning surface

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Access to Sulfonyl Amidines *via* C(sp^2)-*N* Coupling of Trifluoroborate-Iminiums with NFSI

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The syntheses of *N*-sulfonyl amidines often rely on hazardous azide chemistry and transition-metal-catalyzed C–N bond formation. Nonetheless, transition-metal-free approaches for the C-N bond formation remain limited and underexplored. Organoboron compounds have enabled diverse transformations, including transition-metal-catalyzed C-N bond formation using Chan-Lam [1] and aminative Suzuki–Miyaura reaction [2]. We recently reported the first synthesis and transformation of primary trifluoroborate-iminiums (pTIMs) [3], whose unique properties prompted further investigation into their late-stage functionalization to expand their synthetic utility.

We report a novel, azide- and transition-metal-free C(sp^2)-N bond-forming reaction between pTIMs and *N*-fluorobenzenesulfonimide (NFSI), which enables efficient access to unsubstituted *N*-sulfonyl amidines under mild conditions (Figure 1). Aliphatic and aromatic pTIMs underwent the C(sp^2)-N bond-forming reaction with NFSI in the presence of K_2CO_3 and water affording unsubstituted *N*-sulfonyl amidines in good to high yields. DFT calculations revealed dual, base-initiated mechanisms that operate simultaneously. One of them starts by deprotonation of pTIM, whose conjugate base defluorinates NFSI increasing the nucleophilic character of its nitrogen and favoring C-N bond-forming. In the other, the base desulfonylates NFSI generating a highly nucleophilic nitrogen able to attack the C(sp^2) of pTIM to form the new C-N bond. This methodology offers a safe, sustainable route to amidines and expands the scope of transition-metal-free C(sp^2)-N coupling [4].

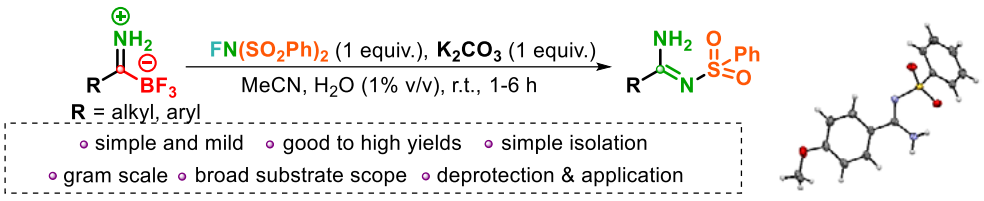

Figure 1: New C(sp^2)-*N* coupling from trifluoroborate-iminiums (pTIMs).

Keywords: C-N bond formation, trifluoroborate-iminiums, NFSI, *N*-sulfonyl amidines, DFT

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XeF_2 and HF coordination to alkali metals in fluoridooxidovanadates(V)

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Complexes of the type $[M^{n+}(XeF_2)_m(AF_x^-)_n]$, featuring XeF_2 as a ligand, form a structurally diverse class of noble-gas compounds [1]. Most involve divalent or lanthanide cations, while the accompanying anions are typically weakly coordinating species, such as AsF_6^- and SbF_6^-. Vanadium trifluoride oxide (VOF_3), a good Lewis acid and fluoride ion acceptor, reacts with metal fluorides to form a range of fluoridooxidovanadate(V) salts [2-4]. In this study, alkali metal fluorides were reacted with VOF_3 in anhydrous HF (aHF), yielding a series of novel compounds, characterized by single-crystal X-ray diffraction and Raman spectroscopy: dimeric-anion salts $Li_2V_2O_2F_8$ and $Na_2V_2O_2F_8$; chain-anion salts $KVOF_4$ and $KV_2O_2F_7$; and HF coordination complexes $[Na(HF)VOF_4]$ and $[K_9(HF)_2V_9O_9F_{36}]$, the latter featuring the largest known oligomeric fluoridooxidovanadate(V) anion $[V_9O_9F_{36}]^{9-}$. Furthermore, reactions of XeF_2 with $Li_2V_2O_2F_8$ and $Na_2V_2O_2F_8$ in aHF solutions resulted in the formation of $[Li_2(XeF_2)V_2O_2F_8]$ and $[Na_2(XeF_2)V_2O_2F_8]$, respectively – rare examples of XeF_2 ligation to alkali metal cations and the first case of coordination to Na^+. Notably, the XeF_2 ligand in both structures adopts a bridging M^+–FXeF–M^+ coordination mode (Figure 1).

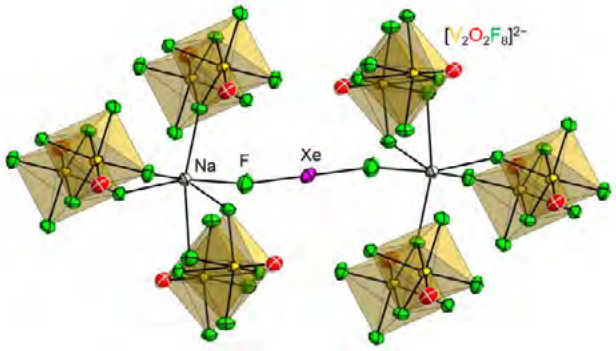

Figure 1: Bridging coordination mode of XeF_2 observed in the crystal structure of $[Na_2(XeF_2)V_2O_2F_8]$.

Keywords: noble-gas compounds, xenon, fluorides, alkali metal, crystal structure

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Preučevanje priprave mezoporoznega Al_2O_3 z metodami termične analize

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Mezoporozni Al_2O_3 odlikuje dobra kemijska, mehanska in termična stabilnost, zato se uporablja na področjih katalize, adsorpcije in senzorike [1]. Izbira sinteznega postopka in variacija sinteznih parametrov vpliva na lastnosti pripravljenega materiala kot so velikost delcev, njihova orientacija, premer kanalov por in njihova periodika.

V predavanju bo predstavljena uporaba raznovrstnih metod termične analize - termogravimetrije, sklopljene z analizo sproščenih plinov (TG-MS) ter diferenčne dinamične kalorimetrije (DSC) - ki smo ju uporabili kot eno od metod karakterizacije za preučevanje priprave mezoporoznega Al_2O_3 ter prehoda v termodinamsko stabilen α-Al_2O_3. Uporabili smo dve različni sintezni poti. Pri hidrotermalni metodi smo preučevali vpliv različnih etanolaminov (mono-, di- in trietanolamina), ki so kot bazični reagent omogočali reakcije hidrolize in kondenzacije, variirali pa smo tudi pH reakcijske zmesi [2]. XRD analiza termično neobdelanih vzorcev je pokazala nastanek delno kristaliničnega γ-AlO(OH), pri materialih, sintetiziranih s trietanolaminom, pa še kristaliničen trietanolamin hidroklorid. Njegova prisotnost je bila razvidna tudi iz ozkega endotermnega signala v DSC krivulji, značilnega za tališče te spojine. Potek termičnega razpada je bil za vse tri vzorce podoben, γ-AlO(OH) se pretvori v mezoporozen γ-Al_2O_3 pri 500 °C. Največjo izgubo mase v temperaturnem območju 200–600 °C je imel vzorec, pri katerem smo kot bazični reagent uporabili trietanolamin, kar je bilo pričakovano, saj je od uporabljenih etanolaminov najšibkejša baza in je bila za uravnavo na določen pH suspenzije potrebna večja količina. Meritve dušikove fizisorpcije so pokazale, da se mezoporoznost ohrani pri temperaturi termične obdelave do 900 °C, iz eksotermne spremembe na DSC krivuljah vseh treh vzorcev pri temperaturi okoli 1250 °C pa smo sklepali, da je prišlo do fazne transformacije v α-Al_2O_3, kar smo potrdili tudi z XRD.

Pri metodi s samourejanjem z izparevanjem topila s solvotermalnim korakom (metoda SA-EISA) smo za preučevanje razvoja strukture glede na temperaturo termične obdelave ravno tako uporabili različne metode karakterizacije: rentgensko praškovno difrakcijo, dušikovo fizisorpcijo, infrardečo spektroskopijo s Fourierjevo transformacijo ter metode termične analize.

Ključne besede: mezoporozen Al_2O_3, hidrotermalna metoda, termogravimetrija, diferenčna dinamična kalorimetrija, rentgenska praškovna difrakcija

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Thermal analysis: a powerful tool in the characterization of nanosized chalcogenides and novel coordination compounds

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Semiconducting nanomaterials such as CdS, CdSe, and CdTe play a vital role in modern electronic devices. CdS and CdSe are of particular research interest due to their favorable optical band gaps of 2.44 eV and 1.74 eV, respectively, while CdTe has proven invaluable in thin-film photovoltaics. Recently, research interest has shifted from binary to ternary materials due to their adjustable band gap range [1]. Among various preparation methods explored, the mechanochemical approach has proven to be a convenient solid-state processing technique, wherein the precursor powders are exposed to repeated fracturing, cold welding, and re-welding in a high energy ball mill. Our group has previously reported on the mechanochemical synthesis of nickel tellurides with various stoichiometries [2]. In this contribution, we present recent advances in the mechanochemical preparation of ternary and quaternary cadmium chalcogenides with general formulas CdS_xSe_y as well as $CdS_xSe_yTe_z$.

In the second part of the presentation, recent advances in the synthesis of copper and cobalt coordination compounds with fluorine- and sulfur-containing pyridine derivatives will be discussed. These compounds have demonstrated significant potential as precursors for the preparation of nanosized metal sulfides *via* the molecular precursor method by controlled thermal decomposition of the coordination compounds with the appropriate metal : sulfur ratio [3].

Powder X-ray diffraction (pXRD) is a key technique for the rapid characterization of reaction progress and product composition. However, a prolonged malfunction of the in-house diffractometer prevented real-time measurements, significantly hindering experimental workflow and necessitating the development of an alternative approach. In this study, a novel methodology employing thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) was established to monitor reaction progress, demonstrating a strong potential for providing fast and reliable data. The results were confirmed by complementary techniques, including Fourier transform infrared spectroscopy (FTIR), dynamic light scattering (DLS), zeta potential measurements, and transmission electron microscopy (TEM) coupled with energy-dispersive X-ray spectroscopy (EDX), as well as externally performed powder and single-crystal X-ray diffraction. Excellent agreement across all methods confirmed the validity of the proposed approach.

Keywords: Ternary cadmium compounds, Mechanochemistry, Coordination compounds, Thermogravimetric analysis, Differential scanning calorimetry.

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Thermally Induced Reversible Martensitic Phase Transition and Self-Healing in Nickel Glycinamide Crystals

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Polymorphic transitions are a well-studied phenomenon with applications in various fields, including pharmacology and materials science [1]. The most common type, reconstructive transitions, generates new polymorphs as randomly oriented domains, often fragmenting the original single crystal into smaller crystallites [2]. In contrast, martensitic transitions, triggered by mechanical or thermal stimuli, involve cooperative atomic, molecular, or ionic movements [2,3]. These transitions—and associated self-healing in molecular compounds—are extremely rare and typically discovered serendipitously, despite their potential for rapid energy transduction [4].

Here, we report the observation of both phenomena in a coordination compound of glycinamide (Glyam), $[Ni(H_2O)_2(Glyam)_2]I_2$ (**1**). Upon cooling, the room-temperature polymorph of this material ($\mathbf{1_{RT}}$) transforms into twinned crystals of the low-temperature polymorph ($\mathbf{1_{LT(twinned)}}$) with the evolution of cracks. Upon heating, it is converted back to $\mathbf{1_{RT}}$ and self-healed into a single-crystal. The crystal structure analysis revealed complex inter- and intramolecular displacements of atoms during the transition [5]. To the best of our knowledge, this is only the second report where a thermally induced reversible martensitic phase transition and self-healing are observed in crystals of a coordination compound.

Keywords: crystal structures, martensitic phase transition, polymorphism, self-healing, twinning

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Študija prehoda α-vijačnica-naključni klobčič z uporabo diferenčne dinamične kalorimetrije

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Toplotna kapaciteta je ena izmed najbolj informativnih eksperimentalno dostopnih termodinamskih količin pri karakterizaciji termodinamskih lastnosti biomolekularnih sistemov. Preko njene statističnotermodinamske definicije lahko denimo ovrednotimo statistično vsoto, kar nam omogoča nadaljnjo izpeljavo ostalih termodinamskih lastnosti sistema (Freire and Biltonen 1978). Kljub njeni dragocenosti pa toplotno kapaciteto raziskovalci le redko analizirajo na absolutni skali parcialnih toplotnih kapacitet.

V študiji bomo predstavili primer analize termogramov z alaninom bogatih α-vijačnih peptidov. Analiza predstavlja še poseben izziv saj je za razliko od globularnih proteinov prehod med naključnim klobčičem in α-vijačnico izrazito nizko kooperativen, kar dodatno otežuje analizo termogramov. Z globalno analizo toplotnih kapacitet na širokem temperaturnem območju smo z uporabo statističnotermodinamskega modela prehoda α-vijačnica-naključni klobčič uspeli dobro opisati potek toplotnih kapacitet α-vijačnih peptidov. Rezultate smo ovrednotili z uporabo verjetnostnega modela na osnovi Bayesove statistike, kar nam omogoča dobro in zanesljivo določitev termodinamskih parametrov prehoda α-vijačnica-naključni klobčič.

Ključne besede: diferenčna dinamična kalorimetrija, peptidi, prehod α-vijačnica-naključni klobčič, termodinamika, Bayesova statistika

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Comparative assessment of CO_2 in waste materials using TGA, TGA-MS and LOI

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Waste ashes and slags, by-products of industrial processes such as incineration and steel production, are of particular interest for carbon capture due to their high alkalinity and reactive mineral phases that enhance their ability to chemically bind CO_2. The carbonation process can increase the utilization of ash or slag by stabilizing these wastes through the conversion of gaseous CO_2 into carbonate minerals (so-called mineral CO_2 sequestration) [1]. In this study, the CO_2 sequestration potential of selected industrial residues is investigated by a comparative analysis using thermogravimetric analysis (TGA), thermogravimetric analysis coupled with mass spectroscopy (TGA-MS) and loss on ignition (LOI).

Two representative raw materials were selected for the analysis: co-combustion ash (CCA; brown coal and biomass) and steel slag (SS; mixture of EAF-S slag and ladle slag). TGA, TGA-MS and LOI are well-established techniques for the characterization of mineral carbonation processes, with TGA in particular being used to quantify the CO_2 content in solid materials. Samples with a particle size below 63 µm were analyzed by TGA, where approximately 10-20 mg of powdered material was placed in an alumina crucible and heated to 1000 °C at a heating rate of 10 °C/min. CO_2 release was quantified by mass loss in a specific decomposition temperature range, which for $CaCO_3$ is around 600-900 °C [2]. The measured weight loss is further interpreted stoichiometrically to estimate the carbonate content. The main limitation of TGA is the possible overlap of mass loss with different phases. In such cases, the use of coupled mass spectrometry (TGA-MS) can improve the accuracy of carbonate quantification. If no TGA or TGA-MS equipment is available, carbonate decomposition can alternatively be assessed using the LOI method. This involves heating 1-2 g of the sample in a laboratory furnace (preferably under an inert gas atmosphere) and quantifying the mass loss within the typical temperature range for decarbonation to estimate the CO_2 or $CaCO_3$ content. However, errors could occur in the determination of LOI if organic compounds are present in the samples. These could be determined using the total organic carbon (TOC) analysis method.

The CO_2 content can be determined using methods such as TGA, TGA-MS, or LOI, each offering different levels of precision and applicability. Among these, TGA-MS provides the most accurate and sensitive measurement, as it not only quantifies the mass loss associated with CO_2 release but also identifies the evolved gases in real time, making it particularly valuable for distinguishing between different carbon forms and gaining deeper insight into the thermal decomposition mechanisms of the sample.

Keywords: Thermogravimetric analysis, Mass spectrometry, Loss on ignition, Biomass ash, Steel slag

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Exploring polymer and surfactant soft-templating in the synthesis of transparent silica monoliths for CO_2 capture

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A potential way to mitigate the increasing amount of CO_2, one the main agents related to climate change, is to capture, controllably release, and store it for later use [1]. The today-available CO_2 capture substances most often rely on toxic and environmentally problematic polyamine resins. As a sustainable alternative, not-functionalized monoliths made from solid naturally abundant materials such as amorphous silicon dioxide or silica, are being investigated for CO_2 capture [2]. In such monoliths, their capability of capturing CO_2 is strongly influenced by their specific surface area, as CO_2 adsorbs to the silica surface. However, a high degree of porosity reduces the mechanical stability of silica monoliths, leading to embrittlement and breaking during handling. The porosity and mechanical stability can be optimised by incorporating soft-templating agents, such as polymers and surfactants. Furthermore, tuning the internal structure of silica monoliths – particularly their average pore size – allows the synthesis of transparent monoliths [3]. This feature is especially advantageous for photothermal (PT) CO_2 desorption applications, where PT-active nanoparticles are incorporated within the silica matrix. In such systems, the transparency of the monoliths permits uniform illumination of all PT-active particles, ensuring their complete activation and a uniform release of the adsorbed CO_2.

In this study we explored the synthesis of transparent, highly porous silica monoliths using polymers and surfactants, as soft-templating agents, to elucidate their effect on the monolith's transparency and porosity. The monoliths were synthesized by sol-gel templating and calcination. Several soft-templating agents were studied, including low- and high-molecular-weight polyethylene glycols, polyvinyl pyrrolidones, and polyvinyl alcohols, starch, microcrystalline cellulose, and surfactants sodium dodecylsulfate and hexadecyltrimethylammonium bromide. The prepared monoliths were examined using gas sorption porosimetry, SEM, and compression tests. We prepared optically and visually transparent monoliths (Figure) with high specific surface area (400 – 800 m^2/g) and small diameter pores (2 – 8 nm). These findings highlight the high potential of transparent silica monoliths for potential future CO_2 capture applications.

Figure. Silica monoliths at ambient light (left) and illuminated by laser light (right), showing their transparency.

Keywords: CO_2 capture, porous, transparent, silica, monoliths

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Acknowledgment: **Project HELICOSS (N2-0389 and J2-6003) and programme P2-0412**

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Estimating Standard Adsorption Gibbs Energy from Corrosion Inhibition Efficiencies

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In corrosion inhibition studies, inhibition efficiency (η) is commonly used as a proxy for fractional surface coverage (θ), enabling the estimation of the standard adsorption Gibbs energy via linear regression of the Langmuir isotherm in the form $c/\theta = 1/K + c$, where c is the inhibitor concentration in the bulk solution and K is the equilibrium adsorption constant. However, this approach frequently encounters two issues. First, both the intercept and the slope are typically fitted, despite the Langmuir isotherm requiring a slope of 1. In practice, the equation $c/\theta = 1/K + mc$ is used instead, where m is the slope. We have recently established a theoretical basis for this equation and demonstrated that it can effectively describe various adsorption models and yield relatively accurate estimates of the standard adsorption Gibbs energy, provided that surface coverages are determined reliably [1]. This leads to the second issue: the $\theta \approx \eta$ assumption is questionable, as demonstrated by Walczak et al. [2]. Hence, a model that maps inhibition efficiency to surface coverage was developed to enable more accurate estimation of the standard adsorption Gibbs energy [3].

Additionally, we showed that any significant deviation from a slope of 1 in the c/θ versus c plot signals non-Langmuir adsorption behavior, caused by inter-adsorbate interactions, multi-site adsorption, surface heterogeneity, or multilayer adsorption. Among these, only attractive inter-adsorbate interactions and multilayer adsorption lead to slopes less than 1.

Keywords: adsorption isotherms, standard adsorption Gibbs energies, corrosion inhibition, surface coverage

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Analytical Sensor Platform for Electrochemical Detection of Pollutants in Flow Conditions

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This paper describes the development, manufacture and performance testing of a miniature analytical sensor platform (ASP) for the electrochemical detection of pollutants under flow conditions. The continuous flow of the analyte through the disposable sensor improves mass transport and leads to high sensitivity. In addition, the compact design enables real-time analysis of the analyte outside the laboratory, making the ASP a fast and cost-effective screening tool for pollution monitoring in remote areas [1].

The ASP was made from low-temperature-cofired ceramic using multi-layer ceramic technology. It has an inlet channel that widens into a cavity designed to accommodate disposable electrochemical sensors (DES), and an outlet channel on the opposite side of the cavity. The flow in the cavity is controlled by an external peristaltic pump [2]. The in-house manufactured DES with electrical connections, counter and reference electrodes from platinum and graphite-based working electrode (WE), all integrated on alumina, are screen-printed and then fired at temperatures of up to 1000°C in an air or argon atmosphere [3].

The finite element modelling software COMSOL Multiphysics was used to evaluate the flow of the analyte in the ASP. The simulated results show that at low flow rates, the streamlines above the WE are parallel. At flow rates above 1 mL/min, we observed regions of recirculating flow, which could impede the mass transport of fresh analyte towards the WE. The critical distance of the analyte was defined as the maximum distance at which analyte diffusion to the WE surface remains feasible. This critical thickness was determined as a function of flow rates and scan rates, based on the mean residence time and diffusion time.

The simulated values were compared with the experimental results. The electrochemical response of DES in an ASP was recorded in a standard solution of potassium ferrocyanide/potassium ferricyanide at room temperature with flow rates up to 10 ml/min and scan rates between 5 and 50 mV/s. We discuss the experimental conditions, namely the range of flow rates and scan rates, at which the analyte supply to the surface of WE in the ASP is sufficient and constant and is reflected in the S-shaped voltammogram with a characteristic limiting current.

Keywords: pollution, fluidic system, electrochemical sensors, low-temperature-cofired ceramic, numerical modelling.

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Surveillance monitoring of the new emerging contaminants – a Case study of the Ljubljanica River

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European Union (EU) Member States (MS) regularly assess waterways for the presence of chemicals considered emerging contaminants, focusing in particular on those that are rarely or never tested [1]. Based on the general water strategy, MS can choose which chemicals they will monitor in their receiving waters. In addition, the legally binding EU Environment Quality Standards Directive (EQSD) and subsequent implementing decisions by the European Commission (EC) introduced Watch Lists (WLs) [1], which mandate the monitoring of selected emerging pollutants across all MS. Their implementation aims to include new priority and priority hazardous substances (PPHS) as a supplement to the actual List of the EQSD, that are determined and likely to be quantified in most European rivers. For a new substance to be included in a WL, a reliable predicted no-effect concentration (PNEC) must be available, along with an appropriate analytical method that has a limit of quantification (LOQ) of at least as low as the PNEC [1]. To assess the EU risk, the EC Joint Research Centre (JRC) proposes that for the dataset, the following criteria must be met: at least 90% of non-quantified substances have PNECs higher than or equal to half of their LOQ [2]. This paper presents an overview of public data on the surveillance monitoring of the Ljubljanica River, conducted between 2009 and 2023. Sampling of surface water was conducted downstream of a treated municipal wastewater discharge point, encompassing the catchment area of Ljubljana [3], which presents a highly urbanised area with the impact of treated industrial and municipal wastewater. The dataset comprises 165 chemicals and 3,088 test results [3], grouped into subcategories based on similar chemical properties and applications. Ninety-seven per cent of the detected concentrations were below the LOQ. However, it was possible to quantify several compounds, including: the antibiotics sulfamethoxazole, trimethoprim, and azithromycin; the anti-inflammatory drug diclofenac; the antidepressant venlafaxine and its metabolite O-desmethylvenlafaxine; caffeine; naproxen; the type 2 diabetes drug metformin and its metabolite guanilurea; industrial chemicals such as 1H-benzotriazole and its metabolites; the surfactant and flame retardant perfluorooctanoic acid (PFOA); the polycyclic aromatic hydrocarbons (PAHs) acenaphthene, fluorene, and phenanthrene; fungicides including 2-nitrophenol, metalaxyl, propiconazole, and azoxystrobin; the herbicides metazachlor and flufenacet; and the antiseptic 2-methoxyphenol. The Slovenian Environmental Agency forwards to the EC only the data regarding the actual WL for final consideration and decision on the selection of additional PPHS [1,2].

Key words: emerging contaminants, Ljubljanica River, priority and priority hazardous substances, Watch list.

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The role of acidolysis on the structure and luminescent properties of Lignin Carbon Quantum Dots

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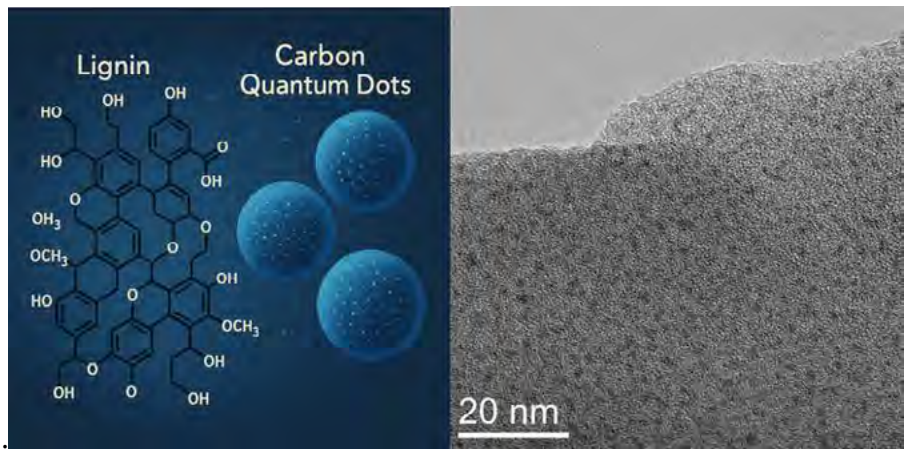
Lignin-derived carbon quantum dots (LG CQDs) are promising nanomaterials due to their structural diversity, low cost, and minimal toxicity. However, their complex structural origins from natural lignin remain insufficiently understood, particularly in relation to their luminescent properties. In this study, we investigated the relationship between synthesis conditions, structure, and luminescence of LG CQDs prepared from spruce lignin using a two-step hydrothermal process. By varying the first step conditions of synthesis, acidolysis step—specifically through the introduction of m-aminophenylboronic acid and differing HCl concentrations—we demonstrated that the initial synthesis step plays a critical role in defining the structure and photoluminescence of the resulting CQDs. Our findings reveal that tuned acidolysis can create distinct reaction pathways, yielding LG CQDs with unique luminescent characteristics. This work provides the first direct evidence of how acidolysis parameters influence the structure and function of LG CQDs, offering new insights for the targeted design of lignin-based quantum dots.



Scheme 1. Representation of lignin structure and structure of LG CQD with TEM image of selected carbon quantum dots

Keywords: Spruce biomass, lignin, carbon quantum dots

The authors gratefully acknowledge the financial support from the Slovenian Research Agency (ARIS) – research core funding grants P1-0134, P2-0423, P2-0089 and P1-0418, research project J2- 50061, and Young Researcher Grant to J.H.). K.E.P., M.Sz. and L.M. acknowledge the support from National Science Center Poland under UMO-2023/05/Y/ST5/00013 project.

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Advancing Divertor Materials: W_2C-Reinforced Tungsten for Fusion Reactors

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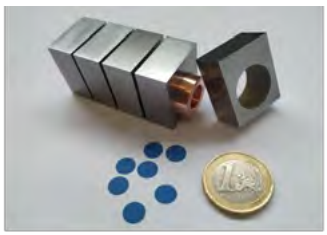
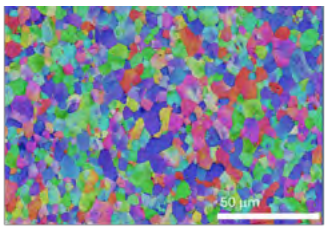
Fusion is considered one of the most promising sources of clean and sustainable energy for the future. One of the key bottlenecks in the development of fusion power plants is the selection of materials for the thermally most heavily loaded components of fusion reactors (divertors). Currently, tungsten is considered as the material of choice for the divertor application of fusion power plants due to its intrinsic thermo-physical properties. However, one main drawback is the recrystallization induced reduction of its mechanical properties at elevated temperatures. Therefore, the aim of the conducted research was to improve the material properties to be able to resist especially the high thermal loads imposed on the divertor during operation.

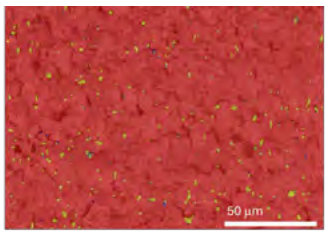
We will show that the particle reinforcement of fusion-relevant tungsten through the incorporation of tungsten sub-carbide W_2C particles at the grain boundaries is demonstrated to be an effective way of eliminating the oxygen present in the starting powder without subjecting it to the hydrogen atmosphere at elevated temperatures. At the same time the densification is being promoted, composite's microstructure is being strengthened and flexural strength at room and high temperatures is increased when compared to the pure tungsten [2]. While higher concentration of W_2C particles lead to the refined grain sizes and higher hardness, low concentration (2-3 wt%) of W_2C particles dispersed in isotropic W matrix displayed the DBTT between 200 and 400 °C. To further decrease the DBTT and increase the fracture toughness of W-W_2C composites, the as-sintered pellets were additionally exposed to compression deformation at elevated temperatures to induce the shape anisotropy of grains. The grain elongation hinders crack propagation along the grain direction, improving fracture toughness in that direction.



W-W_2C composite in the form of a monoblock attached to a cooling pipe



EBSD map showing local crystal orientation distribution using a standard IPF coloring scheme.



EBSD phase map showing phase distribution (red = W, yellow = W_2C)

Keywords: tungsten composites, tungsten carbide, fusion materials, anisotropy

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Development of preceramic polymer-filled filament for additive manufacturing of SiC

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Silicon carbide (SiC) is a widely used ceramic material in the chemical industry due to its chemical inertness and high-temperature stability. Producing such materials using conventional methods—especially for complex-shaped components—is challenging and highly energy-consuming. Additive manufacturing offers an attractive alternative for production of complex shaped ceramics. However, challenges related to binder removal and high temperatures required for densification (1600-2000 °C), hinder its widespread adaptation. The use of preceramic polymers (PCPs) as ceramic precursors provides an economical and practical solution within AM processes. Due to their thermoplastic nature, enabling the use of existing polymer shaping techniques, combined with a low-temperature pyrolysis required to form a ceramic, they can serve as non-sacrificial binders in AM processing [1, 2].

In this work, the effect of preceramic polymer as a major component of the binder system on the development of SiC-based filaments suitable for AM was evaluated. Mixtures of 40-50 vol.% of β-SiC powder with thermoplastic binder composed of preceramic polymer polymethylsiloxane (SMK) and ethylene-vinyl acetate (EVA) in different SMK: EVA ratios were homogenised and extruded into 1.75 mm diameter filaments suitable for the AM process of fused filament fabrication (FFF).

The printability of the filament was determined by its melt viscosity and flexibility. As expected, melt viscosity increased with SiC content, reaching the maximum printable limit at 44 vol.% of SiC. Conversely, increasing the SMK content in the binder reduced the filament's flexibility, making it more difficult to handle. Binder burnout and pyrolysis experiments were conducted at 700, 1000, and 1500 °C in an argon atmosphere. In comparison to conventional SiC processing (without PCP), significantly lower temperatures were sufficient to form a ceramic composite in which amorphous SiOC matrix, formed from SMK, bonded passive SiC filler powder. The final ceramic product showed minimal shrinkage (< 5%) and no significant defects. Flexural strength was found to depend primarily on the amount of SMK in the formulation. Maximal flexural strength of 120 MPa was obtained for composition containing 42 vol.% SiC and SMK:EVA ratio of 65:35, after pyrolysis at 1000 °C.

The results demonstrate that by using preceramic polymers, it is possible to produce filaments suitable for FFF that yield ceramic components with sufficiently high mechanical properties for potential use as catalyst support in chemical industry applications. Moreover, these properties can be achieved at relatively low pyrolysis temperatures, making the process more energy-efficient.

Key words: silicon carbide, preceramic polymer, ceramic composite, fused filament fabrication

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Synthesis and Characterization of W-type $SrZn_2Fe_{16}O_{27}$ Ferrites

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The hard-magnetic W-type $SrZn_2Fe_{16}O_{27}$ ferrites are known for their superior magnetic properties and thermal stability, making them significant candidates for high-frequency and microwave applications. In this study, W-type $SrZn_2Fe_{16}O_{27}$ ferrites were prepared by sol-gel technique followed by auto-combustion [1] and calcination. For this purpose, zinc nitrate, strontium nitrate, and ferric nitrate were taken in stoichiometric ratios as precursors, and citric acid was added for chelation, followed by ammonia for neutralization of pH. The gel obtained was subject to auto-combustion followed by calcination at temperatures 1200, 1300 and 1400°C for 1-4 h to investigate phase formation, composition and crystallinity. The influence of calcination temperature on phase composition, morphology and magnetic properties was investigated. The formation of W-type $SrZn_2Fe_{16}O_{27}$ ferrite phase after calcination was confirmed by X-ray diffraction (XRD). Morphological analysis by SEM revealed an increase in particle size with calcination temperature and time. The magnetic measurements by VSM showed dependence of magnetic properties on calcination parameters due to their significant effect on particle size and phase composition. The present study provides insights into controlled synthesis and structural optimization of W-type ferrites as magnetic materials.

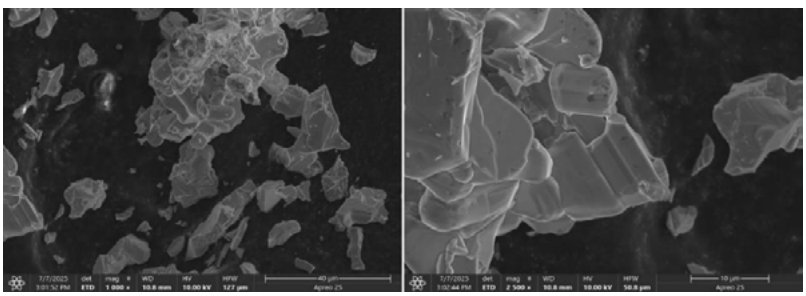

Fig. 1. Microstructure (SEM) of W-type $SrZn_2Fe_{16}O_{27}$ ferrite powder obtained after calcination at1300°C for 2h

Keywords: W-type Ferrites, Magnetic Materials, Sol-gel Synthesis, Calcination.

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BEETHOVEN Funded by the European Union Grant Number: 101129912

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SLOVENSKI KEMIJSKI DNEVI 2025

31ST ANNUAL MEETING OF THE SLOVENIAN CHEMICAL SOCIETY

Slovensko kemijsko društvo
Slovenian Chemical Society

17.-19. SEPTEMBER 2025

ORAL PRESENTATIONS

STUDENT PAPER CONTEST

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Probing the Impact of Mass Transport on Meniscus Electrochemistry by Time-Resolved Operando X-ray Photoelectron Spectroscopy

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Ambient pressure X-ray photoelectron spectroscopy (APXPS) combined with the dip-and-pull method has been thought of as a method particularly suitable for operando studies of electrochemical systems. APXPS probes the electrode/electrolyte interface through the meniscus, whereas electrochemistry collects signals from the meniscus and in bulk electrolyte. Mass transport in the meniscus is not the same as in the bulk electrolyte and the exact impact of mass transport differences on the meniscus electrochemistry is unknown. The difference between the meniscus and the bulk electrolyte mass transport and its impact on the meniscus mass transport are systematically investigated in this work by simultaneously conducting time-resolved APXPS and chronoamperometry for two types of electrochemical processes: capacitive and faradaic. Experiments are conducted on a model system consisting of a gold electrode and carbonate electrolyte. Moreover, experiments are complemented with simulations based on a purposefully constructed transmission line model. A significant meniscus resistance is observed and the ensuing iR drop is shown to have a large influence on the meniscus electrochemistry. Specifically, the large iR drop during faradaic processes results in two to three orders of magnitude slower rate of faradaic processes in the meniscus as opposed to the bulk electrolyte. Based on the gained understanding of the meniscus electrochemistry, we suggest an experimental practice to quantify the iR drop and propose possible remedies for experiments where any impact of the iR drop must be avoided.[1]

Keywords: mass transport limitations, dip-and-pull, electrochemistry, interfaces, ambient pressure

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Operando electrochemical impedance spectroscopy for rechargeable metal anode-based batteries

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Rechargeable metal anode-based batteries have gained enormous attention in both academic and industrial research due to their potential to store more energy compared to systems that use carbon-based anodes. However, achieving reliable and long-lasting metal anode-based batteries requires a deep understanding of the challenges posed by the metal electrode's chemically reactive, non-blocking, and mechanically unstable interfaces and interphases and strategies to address or overcome these issues. Therefore, the interfaces and interphases of metal anodes in batteries need to be closely monitored and understood in order to control battery life during cycling and electrochemical aging. Electrochemical impedance spectroscopy (EIS) is a valuable measurement tool that is widely used to study interfaces and interphases of metal anodes in batteries. EIS, however, requires electrochemical processes to behave as linear time-invariant systems, but these processes are inherently nonlinear and influenced mainly by the state-of-charge of the metal anode-based battery. As a result, EIS is limited to analyzing linear dynamics at fixed operating points under steady-state conditions, making it unsuitable for characterizing processes during active states like charging, discharging, or relaxation. An alternative approach is dynamic EIS, where a small excitation signal is applied alongside the direct current used to alter the SOC. This method allows impedance to be measured simultaneously during SOC changes, *i.e. operando* (hence called *operando* EIS), thus avoiding the challenges associated with open-circuit voltage (OCV) EIS measurements [1].

We have used the concept of *operando* EIS in the following areas in particular: *i)* Li metal batteries, where we have shown that *operando* EIS (by characterizing interphases) can explain the discrepancy between the poorer performance of Li metal in contact with localized high-concentration electrolytes (LHCEs), which have a high Li^+ transport number (t_{Li^+})[2] and *ii)* Mg metal batteries, where *operando* EIS reveals more information about the electrochemical processes occurring on Mg anodes in contact with liquid electrolytes.

Acknowledgments

This work has received funding from the European Union Horizon 2020 research and innovation PhD program DESTINY under grant agreement No. 945357. Co-financing from the Slovenian Research Agency ARIS (core program funding P2-0423) is acknowledged.

Keywords: Li and Mg metal Batteries, EIS, Electrolytes, and Electrolyte/electrode interaction.

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From interest to performance: A comparative study of gender, grade level and different levels of chemistry competition

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The gender gap in science achievement is evident from an early age and becomes more pronounced with higher levels of education, as reflected in participation in competitions. While no significant gender differences were observed at national levels of competition, the proportion of girls in the International Chemistry Olympiads was markedly low, while boys were more likely to participate and perform better. The fact that girls are significantly less likely to be among the top performers in chemistry competitions contributes to their low representation in further scientific careers [1]. Students perceive chemistry as an interesting but challenging subject, involving many formulas and terminology. Students who choose to study chemistry have a more positive attitude towards the subject, especially with regard to its interest and motivation. Support from teachers and parents, along with the connection between chemistry and future careers, are key factors in students' decisions to pursue the subject further [2]. The aim of this study is to investigate the range of achievement in chemistry competitions, whether gender differences in achievement occur and what attitudes competitors have towards chemistry.

The research is based on a causal-non-experimental method of educational research, using a combination of qualitative and quantitative research approaches. The sample is non-randomised and purposive, the data for the study were obtained in cooperation with the Institute of Technical Culture of Slovenia. To compare achievement and gender, the sample consists of 32087 students who participated in a chemistry competition between the school years 2021/22 and 2024/25. Of these, 43.7% are boys and 56.3% are girls. 56% of the pupils are in grade 8 of primary school and 44% are in grade 9. Analysis of the pupils' performance shows that the range of results was largest at school level (0-100%), with lower medians (e.g. 50.18%). At regional level, the ranges were narrower (e.g. 31.11-100%) and the medians were higher (e.g. 70.66%). At national level, the results were even more concentrated (e.g. 51.11-96.67%), with the highest medians (e.g. 77.32%). The trend shows that as the level of the competition increases, the average performance increases and the ranges decrease. In the chemistry competitions, boys achieved higher average results (M = 57.50%; SD = 20.33) than girls (M = 55.00%; SD = 19.71). The Mann–Whitney U test showed statistically significant differences between the sexes in four levels; school level in 8th grade (Z = - 2.520; p = .012), regional level in 8th grade (Z = - 4.362; p < .001), school level in 9th grade (Z = -5.358; p < .001) and national level in 9th grade (Z = -2.075; p = .038). The 370 students who took part in the National Chemistry Competition 2025 expressed a high interest in chemistry on average on a Likert scale (M = 4.20; SD = .47), with 92% indicating that they had good grades and 95% that they were interested in chemistry. The least interest was expressed in the item on doing chemistry in leisure time (M = 3.02; SD = 1.17). There was a statistically significant difference in interest between classes (t = 2.800; p = .005), with eighth graders expressing higher interest, but not between genders (p = .940) or regions (p = .290). The results thus offer insight into gender differences and achievements and may contribute to understanding the factors that influence students' interest in chemistry.

Keywords: chemistry competition, elementary school, achievements, gender, individual interest

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Achievement, motivation and future study decisions of secondary school students in a national chemistry competition

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Chemistry competitions help to build an in-depth knowledge in the field of chemistry. Participants attribute value to competition based on enjoyment and interest, achievement and utility [1]. According to the existing literature, participants' performance in the competition is influenced by their own expectations, parental and teacher support, and gender stereotypes [2]. Our study is based on a non-experimental method with a quantitative research approach. A secondary analysis of the database of the Slovenian Association for Technical Culture (ZOTKS) was conducted, which contains demographic and performance data of 5302 males and 6036 females aged 15 to 19 years from 1st to 4th grade of secondary school who participated in a chemistry competition in the school years 2021/22 to 2024/25. The sample is non-randomised and purposive. The Kolmogorov-Smirnov test ($p < .001$) showed a non-parametric distribution of the data. The Mann-Whitney test is statistically significant ($U = 13927310.5$; $p < .001$). We observe statistically significant differences between female and male students in terms of performance in the chemistry competition in the school years 2021/22 to 2024/25. The data can be generalized to the population in which males ($\bar{x} = 53.47\ \%; \mathrm{SD} = 24.00\ \%$) perform better in the chemistry competition than females ($\bar{x} = 48.14\ \%; \mathrm{SD} = 22.75\ \%$). The second part of the study is based on a questionnaire completed by 305 participants aged 15 to 19 after the 2025 national chemistry competition. The sample is non-randomized and purposive. The most frequently chosen reasons for participation were interest in chemistry ($N = 248$), good grades in chemistry ($N = 129$) and encouragement from the teacher ($N = 67$). A third of the students with good grades cited encouragement from the teacher as the reason for participation. There was a weak but statistically significant positive correlation between the variables *"good grades"* and *"encouragement from the teacher"* ($r = .219$; $p < .001$). Participants who chose the answer "other" most frequently cited the Zois national scholarship for special achievement as the reason for their participation ($N = 28$). Of those who completed the survey, majority ($N = 270$) chose to study science after secondary school. The 4th year students who participated in the Chemistry 2025 competition will enrol in the following degree programs: Faculty of chemistry and chemical technology ($N = 20$), Faculty of mathematics and physics ($N = 14$), Faculty of medicine ($N = 10$), Faculty of pharmacy ($N = 10$), Biotechnical faculty ($N = 3$), the interdisciplinary programme of Computer science and mathematics ($N = 2$), Faculty of natural sciences and mathematics ($N = 2$), Faculty of economics ($N = 1$) and Faculty of mechanical engineering ($N = 1$). These findings provide valuable insights into the motivational and contextual factors that influence students' participation and success in chemistry competitions and highlight the importance of a supportive learning environment in fostering a long-term interest in science.

Keywords: chemistry competition, secondary school students, competition achievement, science career

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Farmakokinetični model fitokanabinoidov

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Teoretična biologija kot interdisciplinarna veda uporablja računalniške modele za preučevanje bioloških procesov, vključno s farmakokinetiko fitokanabinoida tetrahidrokanabinol (THC). Raziskovalci pogosto uporabljajo modele, ki niso dobro primerljivi s človekom, zato model oddelkov omogoča natančnejšo simulacijo presnove THC, njegovih presnovkov THC-OH in THC-COOH ter njihovega izločanja po kajenju. Fitokanabinoidi, kot je na primer THC, nastajajo v smolnih žlezah rastlin rodu *Cannabis* (npr. navadna konoplja (*Cannabis sativa* L.) in učinkujejo na endokanabinoidni sistem preko receptorjev CB1 in CB2, ki sodelujejo pri nevroloških in imunskih funkcijah [1]. THC se po vdihu hitro absorbira v krvni obtok ter distribuira v možgane in adipocitna tkiva [2], njegova učinkovitost pa je odvisna od načina uporabe in posameznikovih lastnosti [3]. Zaradi možnosti zlorabe in varne uporabe fitokanabinoidov je pomembno, da poznamo njihove farmakokinetične in farmakodinamske lastnosti.

Sestavili smo model telesnih oddelkov (ang. compartment model), ki napoveduje distribucijo psihoaktivnih fitokanabinoidov THC in THC-OH v krvnem serumu, krvnih lipoproteinih in adipocitnih tkivih glede na čas. Model sestavljajo trije oddelki: lipoproteini, serum in adipocitna tkiva (kamor smo prišteli še membrane), in pripadajoči koeficient porazdelitev. Model smo opisali kot sistem diferencialnih enačb. Diferencialne enačbe smo vstavili v program Python in jih rešili z numerično metodo Runge-Kutta, RK45. Začetni pogoj in dinamične koeficiente smo dobili iz eksperimentalnih podatkov z iterativnim numeričnim reševanjem sistema navadnih diferencialnih enačb. Postopek smo ponavljali tako dolgo, da smo dobili podatke, ki so kar najbolje opisali eksperimentalni potek koncentracije THC v slini pacientov po enem kajenju.

Primerjava je pokazala relativno dobro ujemanje, kar kaže na zanesljivost modela in s tem potrdili vse postavljene hipoteze. Model predstavlja potencialno uporabno orodje za spremljanje časovnega poteka nivoja kanabinoidov v organizmu, kar je uporabno za varnost pri delu in vožnji.

Ključne besede: farmakokinetski model, fitokanabinoidi, THC, sistem navadnih diferencialnih enačb

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Structural Investigations of the XeF_2–PtF_4 System Under Extreme Conditions

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More than 60 years ago, Neil Bartlett's seminal experiment, in which he oxidised the noble gas xenon with platinum hexafluoride, reverberated within the scientific community, effectively dispelling the long-held belief that noble gases are incapable of forming chemical compounds [1]. However, the product of this interaction, $XePtF_6$, has hitherto evaded comprehensive chemical characterisation, mainly due to its amorphous nature. Subsequent investigations have established that the compound contains tetravalent platinum and can thus be represented as $XeF_2 \cdot PtF_4$ and several structural models have been proposed [2,3]. To gain new insights into the structure of $XeF_2 \cdot PtF_4$, as well as the chemistry of the XeF_2–PtF_4 system in general, we have investigated its behaviour under high-temperature and high-pressure conditions using the laser heated diamond anvil cell (LH-DAC). Synchrotron-based X-ray microdiffraction measurements were performed on laser-heated samples (T > 3000 K) compressed to pressures ranging from 4.5 to 14.3 GPa, yielding several hitherto unobserved crystal structures. Additionally, Raman spectroscopy and quantum chemical calculations were employed to supplement this investigation.

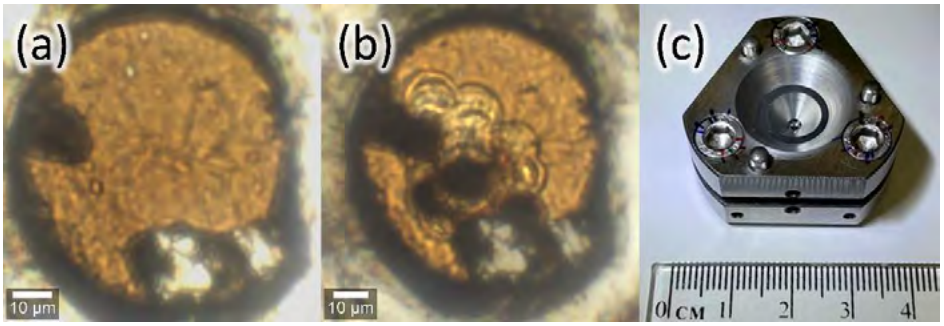

Figure 1: (a), (b) Sample chamber of a DAC containing $XeF_2 \cdot PtF_4$ pressurized to 14.3 GPa before and after laser heating, respectively. (c) Merrill-Bassett type DAC used in one of the experiments.

Keywords: noble-gas compounds, high-pressure crystallography, laser heating

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Synthesis and characteristics of zinc(II) picolinato coordination compounds

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The impact of diabetes mellitus on society highlights the need for novel therapeutic strategies. Certain metal ions, including copper(II), vanadium(IV) and zinc(II), have demonstrated antidiabetic effects, with zinc being particularly significant due to its involvement in various biological processes [1]. However, the bioavailability and efficacy of Zn(II) compounds are critically dependent on their chemical form [2]. Complexation with organic ligands offers a powerful approach to modulate these properties and enhance their therapeutic potential.

Inspired by the promising antidiabetic activity observed in previous coordination compounds with picolinato ligands [3,4], we designed and synthesized a library of novel picolinic acid derivatives. Modifying pyridine-2,6-dicarboxylic acid, we introduced amine functional groups to the initial scaffold. These derivatives were subsequently complexed with zinc(II) ions, and the resulting materials were characterized. Solution studies were conducted to elucidate the behavior of these complexes in relevant media. Single-crystal X-ray diffraction of the obtained crystals revealed a variety in ligand binding to the zinc(II) center, highlighting the influence of the ligand structure, pH, and zinc precursor on the final complex architecture.

Keywords: zinc coordination chemistry, crystallography, solution studies

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Synthesis and characterization of Cu and Ni coordination compounds with XeF_2 as a ligand and RuF_6^- as a weakly coordinating anion

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Noble gases were long considered completely unreactive until, in 1962, Neil Bartlett synthesized the first noble gas compound, $XePtF_6$ [1]. Within less than a year, several new xenon compounds were synthesized, including XeF_2 [2]. XeF_2 can act as a Lewis base by coordinating to a metal center. $[Ag(XeF_2)_2]AsF_6$ was the first synthesized coordination compound with XeF_2 as a ligand [3]. This was followed by the synthesis of numerous new compounds of the general formula $[M(XeF_2)_n](AF_6)_m$, where M is the metal center and "m" its oxidation state, "n" the number of coordinated XeF_2 molecules, and AF_6^- a weakly coordinating anion (WCA) [4]. The synthesis of these compounds involves two steps. In the first step, $M(AF_6)_m$ is prepared. By reacting MF_2 (M = Cu, Ni), Ru, and F_2 in anhydrous HF (aHF) under UV light, $Cu(RuF_6)_2$ and $Ni(RuF_6)_2$ were synthesized. Crystallization was successful only in the case of $Cu(RuF_6)_2$, which crystallizes in the triclinic space group $P\bar{1}$, where CuF_6 and RuF_6 octahedra are linked by shared fluorine atoms forming slabs. In the second step, XeF_2 is added to $M(AF_6)_m$, displacing the weakly coordinated AF_6^- anions in the coordination sphere. XeF_2 was added to $M(RuF_6)_2$ (M = Cu, Ni) in a 2:1 molar ratio and in excess. In the first case crystallization of the reaction products led to the formation of $[M(XeF_2)_2](RuF_6)_2$ (M = Cu, Ni) crystals. The crystal structures of these two compounds belong to the monoclinic space group $P2_1/c$. The metal center is coordinated by two non-bridging XeF_2 molecules and four bridging RuF_6^- anions, which connect neighboring metal centers to form chains. In the case of an excess of XeF_2, crystals of $[M(XeF_2)_6](RuF_6)_2$ (M = Cu, Ni) were obtained. $[Cu(XeF_2)_6](RuF_6)_2$ crystallizes in the triclinic space group $P\bar{1}$, while $[Ni(XeF_2)_6](RuF_6)_2$ in the trigonal space group $R\bar{3}$. In both cases, the crystal structure consists of homoleptic cations $[M(XeF_2)_6]^{2+}$ and discrete RuF_6^- anions. By combining different metal cations and WCAs, we want to deepen our understanding of the behavior of XeF_2 as a ligand in coordination compounds.

Keywords: Copper, Nickel, Xenon(II) Fluoride, Ruthenate

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Three-component iron-based catalysts for sustainable CO_2 conversion into light olefins

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Nowadays, global concerns over the rapid anthropogenic increase in carbon dioxide concentrations have spurred the development of CO_2 utilisation technologies. Such technologies provide a fresh view on carbon dioxide as an economical and renewable carbon feedstock [1]. Among the various chemicals which can be produced from CO_2, light alkenes attract special attention thanks to their widespread use as industrial precursors [2]. Iron-based materials have emerged as promising heterogeneous catalysts for CO_2 transformation into olefin hydrocarbons, owing to their natural abundance, low cost, robust catalytic activity, stability, and tunable surface properties [3].

In this work, we investigate a series of potassium-promoted iron-based K-Fe-M oxide catalysts (where M is Zn, Co, Mn, or Cu) for the CO_2 hydrogenation to light olefins. Each catalyst was synthesised via a co-precipitation technique, followed by washing, drying, impregnation with potassium nitrate, and calcination. Catalytic performance was tested using a packed-bed tubular reactor. Detailed characterisations including N_2 physisorption, X-ray diffraction, scanning electron microscopy, and energy-dispersive X-ray analysis were carried out to correlate structural features with activity and selectivity.

Among the series, the 3K-Fe-5Co catalyst (K : Fe : Co = 0.03 : 1 : 0.5 molar ratio) exhibited both the highest CO_2 conversion of 32 % and light alkenes fraction of 54 % within the gaseous products. This enhanced performance is attributed to a uniform dispersion of active phases, close interaction between Fe and Co species, and increased surface basicity. Overall, our findings highlight the critical influence of catalyst composition on CO_2 conversion efficiency and olefin selectivity, providing valuable guidance for the design of iron-based catalysts aimed at sustainable CO_2 valorisation.

Keywords: CO_2 hydrogenation; light olefins; heterogeneous catalysis; iron-based catalyst; CO_2 Fischer-Tropsch synthesis

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Magnetic heating assisted methanol synthesis from carbon dioxide and hydrogen

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Methanol is the simplest aliphatic alcohol, with the chemical formula CH_3OH. It is a light, colourless and flammable liquid and is used as a solvent, fuel and energy storage medium. More than 20 million tons of methanol are produced every year, which is mainly used as a precursor for other basic chemical substances. These include formaldehyde, acetic acid, methyl tert-butyl ether, methyl benzoate, etc. [1]. In addition to its traditional applications, methanol is receiving increasing attention in Power-to-X (PtX) technologies – a series of processes that convert excess renewable electricity into chemical energy. In this context, methanol serves as an energy carrier and is produced from captured CO_2, and H_2 obtained by water electrolysis. The synthesis of carbon-based fuels increases energy density and enables seamless integration into the existing fuel infrastructure. Thus, methanol is a promising chemical for the storage and transportation of renewable energy in a low-carbon economy. [2]

In this study, methanol synthesis was performed using magnetic heating with a nanocomposite material consisting of CoFe nanoparticles encapsulated in a silica-alumina shell. The preparation was carried out in a two-step process: first, CoFe nanoparticles were precipitated from metal salts by reduction with $NaBH_4$; then the silica-alumina shell was formed around the nanoparticles using tetraethyl orthosilicate (TEOS) and aluminium isopropoxide. After synthesis, the magnetic nanocomposite was reduced in a H_2 stream in a tube furnace to activate the magnetic cores. Subsequently, 20 wt% copper and zinc were co-precipitated onto the silica-alumina shell, yielding the final catalyst for methanol synthesis.

The catalytic experiments were carried out in a fixed bed induction reactor with 200 mg of catalysts and a constant gas flow of 50 ml/min (ratio H_2: CO_2=3:1), a pressure of 30 bar and T 200, 250, 275 and 300°C. At a temperature of 250°C, 0.3 mol% methanol was produced in the gas phase with a very high selectivity. This high selectivity can be attributed to the silica-alumina shell, which acts as a barrier and prevents unwanted side reactions - such as methanation and Fischer–Tropsch synthesis - on the surface of the magnetically heated CoFe cores. These results show that methanol synthesis by magnetic heating is possible and underline the great potential for PtX applications.

Keywords: methanol synthesis, magnetic heating, core-shell nanocomposite, CO_2 hydrogenation

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The Potential of Near-Neutral Deep Eutectic Solvents for Lignin Solubilization and Biocatalytic Applications

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With environmental problems worsening and the urgent need to move away from fossil resources, it is becoming increasingly important to find sustainable ways of using renewable materials such as lignocellulosic biomass in various industries. Lignin is a largely untapped source of aromatic compounds and a promising alternative to fossil feedstocks. Its high carbon and low oxygen content make it suitable for conversion into green chemicals and other high-value bio-based products. However, due to its complex and recalcitrant chemical structure, it is difficult to process and is still predominantly used to generate energy by incineration [1,2]. Depolymerization is one of the main strategies for lignin valorization and can be achieved by electrochemical, thermochemical, or biological methods. White-rot fungi are particularly effective in biological depolymerization, as they secrete extracellular oxidative enzymes capable of modifying and breaking down lignin [2]. Complementarily, deep eutectic solvents (DES) have emerged as effective systems for enhancing lignin solubility and supporting enzymatic activity, providing a dual approach for lignin processing [3].

In our study, we investigated DES, tunable green solvents formed by mixing hydrogen bond donors and acceptors in specific molar ratios, as agents for the mild solubilization of lignin. Lignin was isolated from beech sawdust using the organosolv method [4] and various near-neutral DES formulations (pH 6–7) were tested for their solubilization capacity. Several systems allowed mild yet efficient lignin dissolution at low temperatures, avoiding the use of harsh or acidic conditions. We also investigated the influence of different molar ratios between hydrogen bond donors and acceptors in the DES and found that optimizing this ratio can significantly improve lignin dissolution. Additionally, to evaluate biological compatibility, we performed preliminary agar well diffusion assays with the ligninolytic white-rot fungus *Pleurotus ostreatus*. Selected DES did not inhibit mycelial growth, indicating their potential suitability for integrated lignin solubilization and fungal conversion. This combined approach shows a promising route for lignin valorization and supports the development of sustainable bioprocesses in line with the principles of green chemistry and circular economy.

Keywords: lignin solubilization, deep eutectic solvents, fungal biocatalyst, green chemistry

Acknowledgments: This research was funded by grants from the Slovenian Research Agency for research programs P2-0152 and P4-0077 and research projects L2-50050 and NC-24002.

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Encouraging high school students' interest in polymer chemistry through the context of firefighter protective clothing

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Although polymers and surface-related phenomena such as wettability, hydrophobicity, and surface tension are included in high school science curricula, they often remain abstract and disconnected from students' everyday experiences. This study investigated whether presenting these concepts using the real-life case of firefighter protective clothing could increase student motivation and engagement. This clothing is a relevant example of how polymers and surface effects are critical to human safety. The outer layers of such garments are typically made of high-performance polymers such as aramids (e.g. Nomex®, Kevlar), often with coatings such as fluorinated finishes to ensure water repellency [1, 2]. These coatings create superhydrophobic surfaces with water contact angle above 150°, mimicking biological surfaces such as the lotus leaf [3]. The teaching module highlighted the scientific principles behind protective textiles and their relevance to real life by combining chemistry, physics and biology. To increase accessibility and engagement, the lesson included natural analogies such as the lotus leaf. Analogies, metaphors, images, knowledge, and past experiences help bridge the gap between abstract science and intuitive understanding [4].

The pedagogical approach was based on problem-based learning with 4th grade high school students. The teaching module involved three stages of student experiments: (1) measuring contact angles using contact angle goniometer to determine the wettability of different textile samples, (2) analyzing contact angles based on the polarity of the solvent, and (3) estimating surface tension by counting the number of water droplets a coin surface can hold before overflowing. Student motivation was assessed using pre- and post-lesson questionnaires that measured both individual and situational interest. The responses were quantitatively analyzed to assess changes in interest and perceived relevance of the content.

Preliminary results indicate that students showed greater interest and engagement when polymers were taught through an interactive, real-life, problem-based format than through traditional classroom instruction. In particular, the activity promoted an understanding of hydrophobicity, the role of surfactants and the real-life application of polymers in personal protective clothing. A comparative analysis of chemistry textbooks and national curriculum documents also revealed that applied polymer science related to personal protective equipment is underrepresented in Slovenian secondary education. These results underline the value of integrating practical, interdisciplinary and problem-oriented modules into science education.

Keywords: student motivation, polymers, personal protective clothing for firefighters, wettability

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From stability to rupture: simulating the behavior of ultra-thin surfactant films with molecular dynamics

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Ultra-thin films are essential in various applications, including foam stabilization, drug delivery systems, and environmental processes, yet their inherent instability and susceptibility to rupture are poorly understood [1–3]. Film rupture typically starts with the formation of a sufficiently large pore [1,4], which can be described by classical nucleation theory. Given the challenges of experimentally observing this phenomenon [2,4], we turn to molecular dynamics (MD) simulations. Using GROMACS, we simulate pore formation in ultra-thin films, which ultimately leads to their rupture.

Interestingly, our simulations reveal that even films without an intervening water layer exhibit rupture behavior similar to those containing a thin water layer between them. This suggests that pore formation in these ultra-thin films is primarily governed by interfacial properties (such as surfactant packing and edge tension) rather than solvent effects alone. We further attribute differences in the tendency for pore formation and rupture to variations in edge tension and the presence of H–bonding networks within the surfactant monolayers [5]. These molecular factors offer useful handles for controlling surfactant film stability to meet the needs of specific application.

Keywords: foam stability, ultra-thin surfactant films, film rupture, MD simulations, classical nucleation theory

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Developing an Efficient Free-Energy Method by Combining Multiscale Modeling and Multistate Enhanced Sampling

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Free-energy calculations are one of the central themes in computational chemistry. Arguably the most rigorous approaches are methods based on molecular dynamics (MD) simulations. These are often termed "computational microscope" due to the detailed insight into the studied system they provide. This comes at a cost, though, and the attainable accuracy is limited by the available computational resources. In practice, a trade-off between two main sources of error in MD needs to be struck [1]. These are model approximations and insufficient phase-space sampling. The former can be addressed through the use of multiscale modeling, such as quantum-mechanical/molecular-mechanical (QM/MM) schemes [2, 3], enabling a more precise description of the region of interest compared to classical force fields, and potentially capturing important effects such as polarization. Exploration of the relevant phase space, on the other hand, is facilitated by the use of enhanced-sampling techniques, among which multistate methods, such as replica-exchange enveloping distribution sampling (RE-EDS) [4, 5], are most efficient. We introduce a combined multiscale-multistate free-energy method by integrating the established QM/MM scheme with RE-EDS [6], discuss the details of its implementation, and validate it on hydration free energies. The results show that the developed methodology, which is QM-model agnostic, gives converged results within chemical accuracy and can readily be applied to systems poorly described by classical force fields. Furthermore, we highlight the importance of QM-MM model compatibility and quantify the effects of QM method and classical water model selection. This work lays the foundation for the inclusion of any Hamiltonian, including substituting the QM method by a machine-learned interatomic potential (MLIP) and opens up new avenues for further applications to highly polarizable systems and to those for which force field parameters are not available, thus extending the applicability domain of RE-EDS.

Keywords: molecular dynamics simulations, free-energy calculations, multiscale QM/MM modeling, multistate enhanced sampling

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Structural and Dynamic Effects of Fluorination of Alcohols: Insights from MD Simulations and SWAXS

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Fluorinated alcohols, while different from conventional per- and polyfluoroalkyl substances (PFAS), serve as insightful molecular models to study how fluorination alters intermolecular interactions and liquid structure. In this study, we combine molecular dynamics (MD) simulations with small- and wide-angle X-ray scattering (SWAXS) to investigate how systematic fluorine substitution affects the structural and dynamic behavior of alcohols. Using the complemented system approach [1,2], we directly compare simulated and experimental scattering profiles to validate the structural accuracy of the models at the molecular level. The investigation is carried out in two steps. First, we compare hydrogenated alcohols with their trifluoromethyl analogs and observe a suppression of the OH-associated scattering peak [3] and the appearance of a CF_3-driven mesoscopic organization. With increasing chain length, the local environments around hydrophobic segments in fluorinated alcohols become increasingly similar to those of their non-fluorinated counterparts, as indicated by the positions of the scattering peaks. In the second step, we analyze different fluorinated butanol derivatives and find that a higher degree of fluorination is accompanied by lower positions of the scattering peaks and longer correlation lengths between hydrophobic groups, indicating looser packing in the local hydrophobic environment. MD simulations also show that fluorination significantly affects the dynamic properties, including a decrease in self-diffusion coefficients and an increase in zero shear viscosity, which correlates closely with the evolving liquid structure. Overall, fluorinated alcohols provide a tunable platform for the study of PFAS-related phenomena and provide valuable insights into how specific molecular modifications affect structural organization and dynamics — insights that are critical to advance studies of PFAS behavior in the environment and their remediation.

Key Words: Fluorinated Alcohols, Molecular Dynamics Simulations, Small- and Wide-Angle X-ray Scattering, PFAS

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DFT for CO2ER: Powerful tool or misleading guide?

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Density Functional Theory (DFT) is an invaluable tool for studying heterogeneous catalysis, providing atomic-level insight into reaction mechanisms. However, modeling elementary reactions in electrochemical systems presents unique challenges, such as solvation, the influence of electrode potential and the presence of charged species.

In electrochemistry, electric potential drives reactions at ambient conditions. Precise control over selectivity can be achieved by tuning catalyst, potential, current and solvent. CO2ER has been widely explored experimentally, most of ab-initio studies only target catalyst design. However, for realistic reaction modeling accurate representation of both the electrode potential and solvation effects is essential [1] – failure to do so can lead to misleading results. Charge transfer between the electrode and molecular species in the electrolyte demands especially careful consideration.

To study this complex problem, grand canonical DFT calculations were performed using Solvated Jellium Model [2]. Solvation effects were modeled using explicit solvent, continuum models, and hybrid approaches. The performance of the model is evaluated for CO2 electroreduction on different copper surfaces. Ground state energies were used to identify probable reaction pathways, for which transition state geometry and energy were determined. The results highlight the role of solvation, electrode potential and importance of accurate modeling in electrocatalytic simulations.

Keywords: DFT, CO2ER, CO_2 valorization, solvation, grand canonical DFT, transition states

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Differences in surface modification of various iron oxide nanoparticles with pyrocatechol and guaiacol

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We have been investigating the interaction of the iron oxide-based nanoparticles (NPs) with natural chelates from the catechol family. Barium hexaferrite (BHF) nanoplatelets (NPLs) are based on $BaFe_{12}O_{19}$. They are ferrimagnetic and one of the rare examples of permanent nanomagnets. Consequently, they can be used in various applications, including magnetic microwave devices and recorders, and liquid magnetic systems. Contrary, iron oxide NPs of the spinel ferrite type (SNPs; Fe_3O_4 or γ-Fe_2O_3) exhibit superparamagnetic behaviour and can be used in a wide range of applications, from medicine to sensors. The BHF NPLs used in our research were synthesized hydrothermally, whereas the SNPs were coprecipitated with Fe^{2+} and Fe^{3+} ions using a concentrated ammonia solution.

Pyrocatechol (CAT) is the simplest catechol, with the two hydroxyl groups on the benzene ring. Therefore, it may form a monodentate or a bidentate complex with the iron oxide-based NPs. Guaiacol (GUA) is structurally similar to CAT, but with one hydroxyl group exchanged with the methoxy functional group. As a result, it can only form a monodentate complex with the surface of NPs. The surface modification of both iron oxide NPs was prepared in an ultrasonic bath with a concentration equivalent of 10 molecules of complexants per nm^2.

The surface chemistry properties of NPs were characterized with zeta potential measurements, the quantification of ligand mass fractions was determined by thermogravimetric analysis, and the magnetic properties of modified particles were measured with a vibrating–sample magnetometer. One of the remarkable properties of NPs, due to their nano size and high surface-to-volume ratio, is high chemical reactivity. Consequently, NPs are more susceptible to dissolution in comparison to coarser particles. The chemical stability of the NPs was assessed by monitoring the amount of dissolved Fe using inductively coupled plasma–optical emission spectroscopy (ICP–OES).

Keywords: barium hexaferrite, iron oxide nanoparticles, surface modification, pyrocatechol, guaiacol

Acknowledgement

The study was funded by the Slovenian Research Agency through the research core funding P2-0089 and the research projects PR-12336 and J2-60038.

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SiO_2-Fe_3O_4 Hybrid Monoliths for Photothermal CO_2 Desorption

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Elevated CO_2 concentrations disrupt the Earth's carbon cycle, drawing attention to the need for effective carbon management strategies. The widespread adoption of Carbon Capture, Utilization, and Storage (CCUS) technology is hindered by several challenges, The most critical one is the high operational cost, mainly resulting from the energy-intensive capture process (sorption and desorption).

Although considerable research has been devoted to enhancing CO_2 capture efficiency, the development of economically viable desorption techniques has lagged, creating a significant gap in the overall process. (1) For now in already used thermal swing desorption method, the entire compartment containing the sorbents needs to be heated, which is very energy consuming. To optimize energy consumption, one of the promising approaches can be localized heating of the sorbents using photothermal (PT) effect. (2) But the first step is to create hybrid materials, e.g. silica-iron oxide. In this composite silica act as capturing material and iron oxide nanoparticles (IONPs) act as photothermally active material.

Such hybrid monoliths were prepared via two different methods: (a) Sol-Phase Nanoparticle Dispersion (SPND) where IONPs are added to the sol before it undergoes gelation and (b) Spray coating (SC) of IONPs onto the silica monolith. Initial PTE measurements shows that in the case of SPND method, there is not enough rise in temperature when illuminated by power of 0.1 W ($\approx$ 1 sun). This is due to the "dead" IONPs in the core of monolith, which are not illuminated by light. The significant temperature increase was not observed neither when the monoliths were illuminated with higher power of 1W ($\approx$10 sun). Contrary, in the case of SC monoliths, there is a significant increase in the temperature already for monoliths with the lowest coverage and under low power of 1 sun ($\approx$ 0.1W). The SC prepared hybrid monoliths exhibit hierarchical porosity, with pore sizes ranging from 0.5 nm to few tons of micrometres. Their CO_2 uptake reached up to 1.77 mmol/g at 0°C and 0.96 mmol/g at 25°C, which is significantly higher than in the case of pure silica monolith. Thermally programmed desorption revealed that temperature needed for complete CO_2 regeneration is $\approx$100 °C .To investigate the effect of selectively targeting the absorption maximum, PT experiments were conducted using two narrowband light sources: 447 nm, which coincides with the absorption peak of Fe_3O_4, and 808 nm which does not.

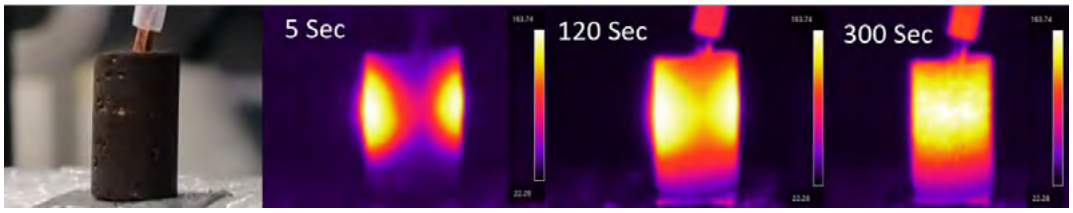

Figure 1: Thermographic images of silica–iron oxide hybrid monoliths heated under narrowband light source.

Keywords: Carbon capture and utilization, photothermal effect, hybrid monoliths, sustainability

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Acknowledgments: Project HELICOSS (N2-0389 AND J2-6003) and programme P2-0412

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Colloidal Stabilization of Magnetic Janus Nanoplatelets in Low-Polar Media

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Janus particles are particles with asymmetric surface properties. Since the term was introduced by Paul de Gennes[1] three decades ago, their unique surface properties have made them a subject of extensive research with promising applications. In our study, we aim to functionalize one face of permanently magnetic barium hexaferrite (BHF) nanoplatelets (NPLs) with electrically polarizable organic ligands. By dispersing so-prepared NPLs in nonpolar solvents, we seek to prepare the first magneto-electric liquid. The magneto-electric liquids are interesting materials for sensors, actuators, etc., since their magnetic properties can be altered with the electric field and vice versa. In order to use magneto-electric liquid in an electric field, NPLs have to be dispersed in a solvent that does not conduct the electrical current. In such solvents, the electrostatic repulsion is not present; therefore, the colloidal stability depends solely on the steric repulsion and its ability to exceed attractive interactions (magnetic dipole interactions and van der Waals interactions) between the NPLs.

In our study, we prepared magnetic Janus NPLs with surface selective hybridization (SSH) technology. BHF NPLs, initially modified with ricinoleic acid (RA), were deposited as a monolayer on a substrate, exposing only one face for further functionalization with polar organic ligands. After functionalization, the Janus NPLs were harvested and redispersed in low-polar solvents. The resulting Janus NPLs were expected to bear RA on one side and a polar ligand on the other, thereby creating asymmetric surface chemistry while, at the same time, enabling steric stabilization in nonpolar media. To study the colloidal stability and identify the cause of instability in such systems, we compared Janus NPLs with isotropic NPLs functionalized uniformly with ricinoleic acid (BHF@RA) or polar ligands. While BHF@RA dispersions remained stable and even displayed ferromagnetic behaviour[2], we found that the SSH harvesting process caused partial desorption of ricinoleic acid. Consequently, Janus NPLs bearing polar ligands on only one face—while the opposite face remained effectively unprotected—lacked sufficient steric stabilization to form stable colloidal dispersions. We studied possible alternative harvesting conditions to realize a stable magneto-electric liquid.

Key words: magnetic nanoplatelets, colloidal stabilization, Janus particles, low-polar media, ricinoleic acid

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Acknowledgment. The authors acknowledge the financial support from the Slovenian Research and Innovation Agency through the research core fundings P2-0089, and P1-0192, and project PR-1012851. The study was partly funded from the MAGNELIQ project. The project has received funding from the European Union's Horizon 2020 Research and Innovation under grant agreement No 899285. The results reflect only the authors' view and the Commission is not responsible for any use that may be made of the information it contains.

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Organic cathode materials for diverse battery applications

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The large-scale deployment of battery technology is driving the research towards the use of more sustainable and less scarce materials. In recent years an alternative to the presently used inorganic cathode materials has emerged in the form of organic cathode materials, which can be made out of abundant raw materials with a lower carbon footprint. Since the traditional inorganic lithium-ion-battery cathodes are reaching their upper theoretical limitations and the room for discovering new intercalation materials is narrow, an alternative pathway of using organic materials could present a future breakthrough in achieving higher energy density and more sustainable post lithium-ion batteries.

The presentation will detail our results concerning the development of novel organic cathode materials. The materials are based on quinone and pyrazine redox-active units and are intended for application in lithium and zinc batteries [1,2,3]. We will discuss their synthesis strategies, which also utilize biomass-derived precursors. Performance metrics will be presented, highlighting active material energy densities reaching up to 860 Wh/kg in lithium batteries and 330 Wh/kg in zinc batteries, figures that represent significant advancements in the field. Furthermore, we will provide an in-depth analysis of the underlying redox mechanisms inherent to these materials.

Keywords: batteries, organic cathode, zinc, lithium, zinc

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Competitive role of anions in LiTFSI-$LiNO_3$ mixed electrolytes: transport-structure relationship

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Novel battery electrode materials, such as lithium/sodium metal and multivalent batteries have been proposed to address ethical and environmental concerns posed by the rapid expansion of Li-ion batteries. In this context, electrolyte design is a key step for practical implementation of new electrode materials [1]. Specifically, mixing of salts with different anions appears as an increasingly promising approach [2].

A notable class of mixed-anion battery electrolytes is based on lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) and lithium nitrate ($LiNO_3$) salts in organic solvents. These electrolytes significantly improve the performance of lithium-sulphur and lithium-oxygen batteries. In particular, it has been shown that the LiTFSI to $LiNO_3$ concentration ratio controls the solubility of sulphur species and the electrochemical stability of the electrolyte, strongly affecting the performance of a battery cell. This effect has been mainly attributed to the effect of the anion ratio on the solvation structure of lithium cations [3].

What remains unclear is the effect of the interplay between $TFSI^-$ and NO_3^- anions on the ion transport through the electrolyte, which strongly impacts battery charging efficiency and lifespan. We perform classical molecular dynamics simulations, supported by electrochemical impedance and Raman spectroscopy measurements, to study how the $TFSI^-$ to NO_3^- anion ratio impacts Li^+ transport in the diglyme-based electrolytes [4]. We show that the anion competition affects both the structure and dynamics of Li^+ solvation, which together contribute to the distinct transport properties of the studied electrolyte and, likely, other mixed-anion electrolytes.

Keywords: electrolytes, batteries, cation-anion association, transport properties, molecular dynamics

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Surface Modification, Magnetic Field and Solvent Effects in Magnetoactive Elastomer Composites

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Magnetoactive elastomers (MAEs) are a class of soft composite materials composed of magnetic nano- or microparticles embedded within polymer matrices, capable of dynamically altering their mechanical behavior in response to external magnetic fields [1,2]. This tunable response makes MAEs highly attractive for applications in soft robotics, adaptive actuators, and vibration damping systems [1–3]. However, limitations in reproducibility and a lack of comprehensive understanding of their structure–property relationship continue to hinder their broader application.

This study investigates the effects of filler concentration, surface modification, solvent environment, and magnetic field exposure during curing on the microstructure and mechanical properties of MAEs based on a polydimethylsiloxane (PDMS) matrix with hexaferrite (HF) fillers. A primary focus is on preventing particle agglomeration and improving both filler distribution and compatibility with the polymer matrix. Surface modification of strontium hexaferrite (Sr-HF) microparticles using dodecylbenzene sulfonic acid (DBSA) slightly reduces agglomeration and enhances distribution. However, the use of 1-butanol as a solvent introduces porosity due to evaporation, affecting the mechanical properties of MAEs. The application of an external magnetic field during curing promotes some alignment of filler particles, in contrast to the random filler distribution observed in samples cured without a magnetic field. Rheological analysis reveals that 1-butanol, when used with scandium-substituted barium hexaferrite (BSHF) fillers, significantly delays curing (from 47 min in pure elastomer to 77 min in the MAE) and reduces crosslink density, thereby softening the polymer network (*G'* reduced from 7400 Pa to 3500 Pa). By systematically analyzing these effects and optimizing surface-modification strategy, this research aims to advance rational design of MAEs with programmable mechanical and magnetic responses.

Keywords: magnetoactive elastomers, hexaferrite, surface modification, soft robotics

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Acknowledgment. This research has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie Actions Doctoral Network MAESTRI (grant agreement No. 101119614), and Slovenian Research and Innovation Agency through the research core funding P2-0089. Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union or the European Research Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.

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Utilization of magnetic heating in bio-based compound processing

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Lately, the global consciousness about the mitigation of fossil fuel use grows. This opens up many opportunities for testing various new energy sources that are more ecological and environmentally friendly. A promising renewable energy source is lignocellulosic biomass which contains natural C5 and C6 sugar polymers. The processing of these sugars results in platform molecules such as furfural, 5-hydroxymethylfurfural (HMF), and levulinic acid.[1,2] Bio-based platform molecules enable the production of different value-added compounds, which can be utilized in the pharmaceutical industry, fuel industry, cosmetics etc.[3] Furfural is one of the most essential platform chemicals due to active groups, such as the aldehyde group and the unsaturated furan ring enable the formation of different value-added chemicals *via* furfural hydrotreatment.[2]

Since bio-based compounds are thermally sensitive and thermally degrade under elevated temperature, the main idea of this work is to overheat the spots on the catalyst surface, while keeping the reaction mixture cooler. Latter could be achieved with the help of magnetically heated catalysis.[4] The catalyst used for furfural hydrotreatment is a magnetic nanocomposite catalyst consisting of iron oxide magnetic core coated by γ-alumina support and decorated with ruthenium nanoparticles as a catalytically active material.[2] Under the influence of the alternating magnetic field (AMF), the catalyst inside the batch reactor system heats up *via* magnetic hysteresis heating, exhibited by ferrimagnetic iron oxide nanoparticles. The switching in the magnetic moment orientation inside the nanoparticles results in the release of energy in the form of heat. A figure of merit for the heat exhibited by the mass unit of material is called the specific absorption rate (SAR).[4] A comparison between magnetically and conventionally heated reactor systems will be presented to gain insight into the kinetics of the furfural hydrogenation reaction under both "local" magnetic heating and "global" heating of the entire reactor with conventional electric heaters.

Keywords: biomass, furfural, magnetic heating, furfural hydrotreatment

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Decarbonizing hydrogen: LCA of magnetically heated methane decomposition

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Catalytic decomposition of methane (CDM) offers a CO/CO_2-free route to hydrogen, producing solid carbon as the only byproduct [1]. Unlike conventional reforming, CDM eliminates the need for downstream carbon oxide separation, making it a promising alternative for clean hydrogen production. One of the most promising pathways to improve CDM viability is through electrification via magnetic induction heating, which enables localized catalyst heating and reduced thermal losses.

In this study, we conduct a life cycle assessment (LCA) of CDM over commercial Fe-Ni-Co and Ni-Cr-Co catalysts operated in an induction-heated reactor. Methane decomposition was performed across a temperature range of 450 to 650 °C, with several catalytic systems demonstrating stable methane conversion exceeding 40% over more than 10 hours. All the catalysts produced carbon nanotubes (CNTs) as the main carbon product, shich is extremely important for economic efficiency of CDM [2] While magnetic induction allows efficient energy delivery, the relationship between supplied electrical energy and resulting catalyst temperature is highly dependent on the material's magnetic and electrical properties [3], making optimization nontrivial.

LCA is employed to assess the environmental performance of the process under different operating conditions and catalyst compositions. Beyond its sustainability relevance, the LCA also provides critical insights into the energy-material interactions in magnetically heated systems, supporting better economic evaluation and reactor design optimization [4]. Both hydrogen and carbon nanotube (CNT) production scenarios are considered, providing a broader picture of the system’s impact and potential value.

Keywords: Catalytic methane decomposition; Hydrogen production; Carbon nanotubes; Magnetic heating; Life cycle assessment

The research was founded by European Union’s Horizon Europe Research and Innovation Programme, under Grant Agreement n° 101069690.

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Application of the Horner–Wadsworth–Emmons Olefination in the Construction of *E*-α,β-Unsaturated β-Boryl Nitriles

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α,β-Unsaturated β-boryl nitriles represent versatile intermediates in organic synthesis, as they are built with multiple reactive sites, including the cyano group, the boron moiety, and the conjugated double bond, which enable a wide range of chemical transformations. To date, only three synthetic methods for the preparation of α,β-unsaturated β-boryl nitriles are known; however, they either rely on palladium catalysts or require high or cryogenic temperatures, all of which are unsuitable for industrial-scale applications, highlighting the need for further investigation [1,2,3].

Since 2010, acylboranes have attracted increasing attention due to their promising chemical properties; however, they remain relatively underexplored to this day [4]. In our research (Figure 1), we focused on potassium acyltrifluoroborates (KATs), which have proven to be excellent precursors for the synthesis of pure *E*-α,β-unsaturated β-boryl nitriles via the Horner–Wadsworth–Emmons (HWE) reaction. Under mild and transition-metal-free reaction conditions, various KATs, such as aryl, heteroaryl, and alkyl derivatives, were stereoselectively and efficiently converted into the corresponding *E*-α,β-unsaturated β-boryl nitriles in good yields (mostly 50 – 80%). The pure *E* isomers were isolated either by precipitation or crystallization, eliminating the need for additional purification by column chromatography. In conclusion, the method's inherent simplicity and scalability emphasize its considerable promise for practical implementation [5].

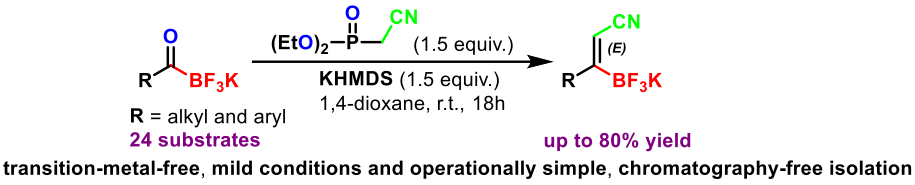

Figure 1: HWE Olefination of Potassium Acyltrifluoroborates

Keywords: *E*-α,β-unsaturated β-boryl nitriles, HWE reaction, potassium acyl trifluoroborates

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Landfilling mining for polyolefins recovery and material utilization

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Legacy landfills are a neglected source of stable polyolefins (HDPE, LDPE, PP), which retain material and calorific value even decades after disposal. This study explores their recovery from baled waste at the CERO Gajke landfill (Ptuj, Slovenia) [1] and transformation into paraffinic waxes via controlled, material-oriented pyrolysis. [2]Emphasis is placed on moderate temperatures (400–500 °C), tailored residence time, heating rate, and inert atmosphere to favour long-chain hydrocarbon formation. [3]

The process follows a radical degradation mechanism involving β-scission and backbiting, enabling wax yields of up to 90 % under isothermal conditions. A light condensate fraction (~135 °C) is also recovered. [4], [5] Sorting data show that ~40 % of excavated waste is plastic-rich, predominantly polyolefin packaging, suitable for pyrolysis after pre-cleaning. [6] The approach offers a scalable route for decentralized valorisation of legacy plastics into high-value waxes, supporting circular economy objectives within the technospheric mining framework. [7]

This research is part of the ARIS-funded project *Mining the technosphere for efficient use of resources and improving state of the environment* (acronym: J7-50228).

Keywords: Legacy landfills, polyolefins, controlled pyrolysis, paraffinic waxes, technospheric mining

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Extracting Magnesium from Slovenian Dolomites

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Although one of the most abundant elements on Earth, magnesium has been categorised as a critical mineral resource by the EU [1]. Due to many desirable properties, the metal itself, its alloys, and its compounds have found varied uses in different industries. Together with potential new applications (e.g., energy storage) [2] the demand for Mg is increasing and putting a strain on its production, which is largely dependent on two energy intensive processes – molten salt electrolysis and thermal reduction [3]. Alternatively, hydrometallurgical processes are being developed to selectively extract and concentrate Mg from its sources [4].

Main magnesium ores are magnesite, dolomite, and talc. Dolomite is chemically $CaMg(CO_3)_2$ and is a common carbonate sedimentary rock that is formed from limestone by cation exchange – a process called dolomitisation. According to the chemical formula dolomite contains 13.18 % of Mg by weight. The surface of Slovenia is covered by sediments and sedimentary rocks, with limestone and dolomite being the most prevalent. Deposits of dolomite cover about 10 % of the territory of Slovenia [5]. Because of its abundance and accessibility, dolomite is an important source of Mg. Slovenian dolomites can therefore be a potential source of Mg.

In our study dolomite samples were collected across Slovenia, from different geological formations and from different geological periods. Elemental analysis was performed with microwave assisted acid digestion and the elemental composition determined by ICP-OES. The samples were found to be very pure dolomite with mass percentages of magnesium close to the ideal value and with almost no impurities. Mg was then selectively extracted from the dolomite by two hydrometallurgical processes – selective leaching and selective precipitation. Using solutions of H_2SO_4, oxalic acid, and tartaric acid Mg was successfully selectively extracted, and a Mg-rich fraction was prepared with improved Mg:Ca molar ratio in favour of Mg. Selective precipitation of Mg from solutions of dissolved dolomite with hydroxide solution resulted in the preparation of a Mg-rich precipitate that contained above 90 % of the present Mg.

Keywords: magnesium, dolomite, selective leaching, selective precipitation, ICP-OES

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Solid-State Structural Characterization of Organic Dihydroperoxides

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Organic dihydroperoxides represent a broad group of molecules with a wide variety of applications. They are used as energetic materials, disinfectants, radical polymerization initiators and valuable oxidants in organic synthesis.[1] Of particular interest are their pronounced antimalarial properties,[2] which have driven significant synthetic and biochemical research progress.

While synthetic methods towards organic dihydroperoxides are well established, structural characterization by X-ray diffraction remains scarce. This is largely due to their sensitivity and potential explosiveness in the solid state, which limit crystallographic investigations. One effective strategy to mitigate this limitation is cocrystallization, which employs non-covalent interactions, especially hydrogen and halogen bonds to stabilize reactive species. Cocrystallization, widely applied in pharmaceutical development, improves solubility and mechanical properties, and has proven particularly useful for stabilizing sensitive materials.[3]

In this work the scope of organic peroxides characterized in the solid state is expanded to include 1,1'-dihydroperoxy(dicycloalkyl)peroxides and *gem*-dihydroperoxides stabilized through hydrogen bonding with Ph_3AsO (Fig. 1).[4] The *gem*-dihydroperoxides were synthesized by the established reaction of selected ketones with aqueous hydrogen peroxide and characterized by low-temperature single-crystal X-ray diffraction.

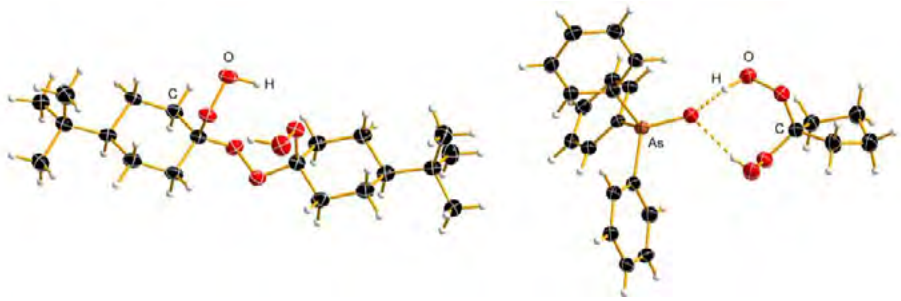

Figure 1. Crystal structure of 1,1'-peroxybis(4-(tert-butyl)(hydroperoxy)cyclohexane) (left) and Ph_3AsO·1,1-dihydroperoxycyclopentane cocrystal (right).

Keywords: organic peroxides, single-crystal X-ray diffraction, cocrystallization, hydrogen bonding

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Salt cocrystals featuring XeF_2 as a hydrogen-bond acceptor

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XeF_2 is a linear, centrosymmetric, and nonpolar molecule whose high solubility in polar and protic solvent anhydrous HF (aHF) [1] is attributed to FXeF···FH hydrogen bonds. This intermolecular interaction also plays an important role in the chemistry of XeF_2, as its reactivity is significantly increased even in the presence of catalytic amounts of HF [2]. However, only a few crystallographically characterized examples of XeF_2 as hydrogen-bond acceptor are known. These include $(H_3O)[AsF_6]\cdot 2XeF_2$ [3], $HNO_3\cdot XeF_2$ [4], and $[Cd(FH)_2(XeF_2)(TaF_6)_2]$ [5], in which either OH···F(Xe) or HF···F(Xe) hydrogen bonds are observed. Another example is the salt cocrystal $(CF_3C(OH)NH_2)[AsF_6]\cdot XeF_2\cdot x$HF [6], where the presence of O/N−H···F(Xe) hydrogen bonding was inferred from Raman spectroscopy.

To investigate the hydrogen-bonding propensity of XeF_2, the salts $(CF_3C(OH)NH_2)[AsF_6]$, $(C_2F_5C(OH)NH_2)[AsF_6]$, and $(C_3F_7C(OH)NH_2)[AsF_6]$ were reacted with XeF_2 in aHF at low temperatures, yielding $(RC(OH)NH_2)[AsF_6]\cdot XeF_2$ salt cocrystals. In all crystal structures, a rare example of an N−H···F(Xe) hydrogen bond (2.667(6)–2.7875(14) Å) is observed. Only in the crystal structure of $(CF_3C(OH)NH_2)[AsF_6]\cdot XeF_2$ (Figure 1) is an O−H···F(Xe) hydrogen bond (2.545(1) Å) also observed, which is shorter than those reported in $(H_3O)[AsF_6]\cdot 2XeF_2$ (2.571(3) Å) [2] and $HNO_3\cdot XeF_2$ (2.690(1) Å) [4].

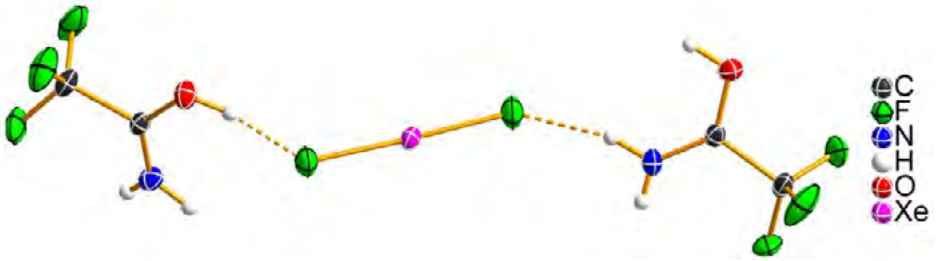

Figure 1: Hydrogen bonds (dashed lines) between XeF_2 and protonated trifluoroacetamide in the crystal structure of $(CF_3C(OH)NH_2)[AsF_6]\cdot XeF_2$ salt cocrystal. Displacement ellipsoids are shown at 50% probability level.

Keywords: noble-gas compounds; hydrogen bonds; superacidic medium; crystal structures;

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Synthesis and Structural Characterization of $[RN{-}Xe{-}F]^+$ Adducts with Malononitrile and Fluoroacetonitriles

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The $[RN{-}Xe{-}F]^+$ adduct cations represent an important family of compounds in which a noble gas is directly bonded to nitrogen. These and similar adducts form when a Lewis acid containing a polarized xenon atom, such as the $[XeF]^+$ cation, is coordinated by a Lewis base bearing a nucleophilic nitrogen atom (Figure 1). To date, adduct cations containing Xe–N bonds have been reported with nitriles (R–CN, where R = H, CH_3, CH_2F, CF_3, C_2H_5, $(CH_3)_3C$, C_2F_5, C_3F_7, C_6F_5), fluorinated heterocycles (e.g., C_5F_5N, 4-$CF_3C_5F_4N$, *s*-$C_3F_3N_3$), and inorganic Lewis bases such as F_3SN, although only a few of them have been crystallographically characterized [1–5].

To expand the structural chemistry of Xe^{II}–N-bonded systems, $[XeF][AsF_6]$ was reacted with malononitrile ($NCCH_2CN$) and a series of fluoroacetonitriles (CH_2FCN, CHF_2CN, and CF_3CN) in anhydrous HF (aHF) at low temperature. The resulting $[RN{-}Xe{-}F][AsF_6]$ adduct cation salts were obtained as single crystals, enabling their structural elucidation by low-temperature single-crystal X-ray diffraction. Low-temperature Raman spectroscopy was employed to further investigate the bonding in these unstable compounds.

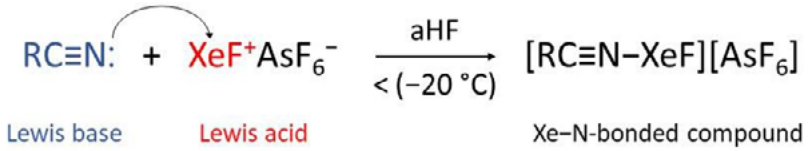

Figure 1. The reaction scheme for the synthesis of Xe–N bonded compounds.

Keywords: Xe–N-bonded adduct cations, crystal structure, single-crystal X-ray diffraction.

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Microscopic protolytic equilibrium of ellagitannins and its influence on the chelation of metal ions

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Tannins are polyphenolic secondary metabolites in higher plants with several beneficial properties (antibacterial, antioxidant, etc.). These properties result from the structural features (multiple phenolic groups) of tannins, which enable them to form complexes with proteins and coordination compounds with metal ions. Understanding the formation of coordination compounds is crucial as it plays a key role in the potential applications of tannins. For example, the chelation of Fe(II) ions (which are essential for bacteria) by tannins is important in agriculture, as tannin extracts are used as a substitute for antibiotics in animal feed. On the other hand, the interactions between tannins and Al(III) ions, which are toxic to plants, lead to the formation of non-toxic coordination compounds. The protolytic equilibrium of tannins strongly influences the interactions between metal ions and tannins, as chelation occurs through deprotonated hydroxyl groups [1][2].

In our work, we investigated the microscopic protolytic equilibrium of methyl gallate (model compound) and ellagitannins (vescalin, castalin, vescalagin, and castalagin). For this, we used a combination of NMR spectroscopy and DFT calculations. From the pH-dependence of ^{13}C chemical shifts, the microscopic pK_a values of most acidic hydroxyl groups were determined for individual aromatic rings of methyl gallate and four polyprotic ellagitannins [3]. The deprotonation positions of the phenolic protons were determined by comparison of experimental and DFT-calculated NMR spectra [3]. We then investigated the chelating ability of the ellagitannins. Using Job's method, we determined the stoichiometries of the coordination compounds of ellagitannins and metal ions (Fe(II) and Al(III)) in the pH range of 5.5–3.5. In the case of the coordination compounds with Al(III) ions, we determined the exact binding position by NMR spectroscopy and additionally confirmed it with DFT calculations. With the information on the number of chelated metal ions per structural group of the ellagitannin, the exact binding position and the dissociation constant of the hydroxyl groups involved in the chelation, we have developed a universal model that can describe and predict the chelation of Fe(II) and Al(III) ions by structural groups of ellagitannins. This model can be used to predict the chelating ability of as yet untested ellagitannins with the same structural groups.

Keywords: ellagitannins, microscopic pK_as, NMR spectroscopy, DFT calculations, Al(III) ions

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Multifunctional Bioaerogels for Wound Healing Applications

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Wound healing is the body's natural response to repair the damaged tissue. This complex biological process involves four sequential, overlapping phases: immediate haemostasis, followed by inflammation, proliferation and maturation [1]. However, in chronic wounds, factors such as bacterial accumulation and oxygen deficiency can hinder the healing process and lead to serious complications [1,2]. To overcome these challenges, we developed biodegradable and multifunctional bioaerogels that can deliver drugs, eliminate bacteria, and oxygenate the wound site simultaneously [3].

The bioaerogels were synthesised from xanthan gum and polylactic acid (PLA) by a conventional sol-gel process followed by drying with supercritical CO_2. Dexamethasone was incorporated as an anti-inflammatory model drug, while sodium percarbonate and calcium peroxide served as oxygen-generating compounds. Two materials with different compositions were produced and characterised. The developed bioaerogels were highly porous and had a high specific surface area (up to 396 ± 8 m^2/g). Swelling and stability studies in simulated body fluid revealed high liquid absorption capacity (up to 67 times their original weight) and a structural stability that was maintained for 72 h. *In vitro* drug release tests showed a controlled release profile of dexamethasone over 24 h, demonstrating the potential for localised, sustained treatment. Antibacterial activity was confirmed against *Escherichia coli* and *Staphylococcus aureus*, with inhibition zone diameters of up to 15.92 mm and 31.07 mm, respectively. *In vitro* biocompatibility tests with mouse fibroblast cells (NIH/3T3) showed excellent cytocompatibility with a cell viability of >90%. Furthermore, haemocompatibility tests with human blood showed no haemolytic activity (lysis rate <2%), indicating the safety of the bioaerogels for biomedical use. Overall, these results underline the great potential of bioaerogels to revolutionise the treatment of chronic wounds.

Ključne besede: aerogel, supercritical drying, wound healing

Reference

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Mechanistic Insights into the Anti-Cancer Effects of Cannabinoids in Colon Cancer Cells

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Cannabis sativa has a long history of use in human health, yet systematic evidence elucidating the mechanistic basis for the anticancer effects of specific cannabinoids is only now emerging, and the exact molecular mechanisms of their activities remain only partially understood. In our previous work, we demonstrated that Cannabis extracts reduce the viability of colon cancer cells in a dose-dependent manner, with minimal effects on non-cancerous epithelial cells at equivalent concentrations [1]. Recent *in silico* studies from our group further revealed novel potential targets for various phytocannabinoids, including cancer-related kinases, using an inverse molecular docking fingerprint approach [2]. Building on these insights, we now explore the mechanistic effects of various isolated phytocannabinoids derived from *Cannabis sativa* on colon cancer cells through a combination of molecular methods using *in vitro* cell models.

We profiled the expression of classical cannabinoid receptors CB1 and CB2, transient receptor potential (TRP) channels, G protein-coupled receptor 55 (GPR55), and peroxisome proliferator-activated receptor gamma (PPARγ) in Caco-2 and HCT116 cell lines using flow cytometry and western blotting. Cell viability in response to 16 cannabinoids was assessed using Alamar Blue assay. To investigate receptor involvement in cannabinoid-mediated effects, we employed receptor-specific antagonists and agonists. In addition, we used multiplex immunoassay to evaluate cannabinoid-induced changes in signaling pathways related to cell growth, proliferation, survival, and apoptosis.

Our results showed that expression patterns of CB1, CB2, TRPs, GPR55, and PPARγ receptors differ between the Caco-2 and HCT116 cell lines. Initial pharmacological studies suggest that these receptors are involved in mediating the anti-cancer effects of cannabinoids, although the extent of their contribution remains to be fully defined. Cannabinoids reduce cell viability in a dose-dependent manner, with neutral (decarboxylated) forms generally showing greater potency than their acidic counterparts. Early signaling analyses point toward both shared and distinct effects of individual cannabinoids on key regulatory proteins involved in cell survival and apoptosis, with cell line-specific variability. These findings suggest a complex, context-dependent mechanism of action and support the therapeutic potential of cannabinoids in colorectal cancer. Moreover, the observed heterogeneity in receptor expression and signaling responses highlights the importance of personalized approaches in developing cannabinoid-based therapies tailored to tumor-specific molecular profiles.

Keywords: Cannabinoids, colorectal cancer, signaling pathways, personalized medicine

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»I'm in charge now!« - Explaining a surge in activity of novel mtKv1.3 leads by charge screening effects

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Mitochondria-targeted therapy has stood out in the past decades as one of the most promising approaches within organelle-targeted therapies in modern drug discovery[1]. Recent clinical setbacks[2] have served as a checkpoint to reassess the state-of-the-art in mitochondria-targeted drug discovery. Among the problems in the current state of mitochondria targeting drug discovery, we have identified the intrinsically bioactive triphenylphosphonium cation (TPP) that, more than 50 years since its discovery, still holds the title of the »golden standard« mitochondria-targeting moiety (MTM) - a molecular fragment that is covalently bound to functional (therapeutic) moieties with the intent of delivering them to the mitochondria. Its pronounced unwanted biological effects have repeatedly been shown to occur[3] wherever it has been used to exclusively accumulate in the mitochondrial matrix. We have thus decided to search for a modern replacement for TPP within the domain of previously seldom researched lipophilic pyridinium cations.

In the last year's SKD conference, we have disclosed the first library of efficient phosphonium-free MTM. Among them was the frontrunner mitochondria-targeting moiety 3,5-diphenylpyridinium (3,5-DPPy) and, since then, several in-vivo studies have begun with its Kv1.3 inhibitor conjugates and other mtKv1.3 inhibitor candidates. The frontrunner MTM has been shown to selectively kill pancreatic cancer organoids, and leave healthy human cells unharmed at timepoints of 10-12h post-treatment. However, the most compelling line of work has been the lead optimization campaign, which aimed to identify more active analogues of 3,5-DPPy and overcome its pronounced solubility issues by finding alternatives with improved thermodynamic solubility. Here, a series of six mtKv1.3 inhibitors that include novel MTM is presented. Upon noticing most promising results so far in terms of potency and selectivity of any novel mtKv1.3 inhibitor in the Resazurin assay, we were encouraged to link the biological properties of the novel MTM to several other—more fundamental—experimentally determined descriptors that were of interest: Crystal structure and electron density (both obtained by XRD), partition coefficient (LogD7.4), and thermodynamic solubility (TS). Among the most interesting findings was 2,5-DPPy, a structural isomer of the previous frontrunner, where a phenomenon of increased activity, attributed to the charge screening by the neighbouring phenyl group, was noticed. The remaining analogues followed the pattern and were consistent with the charge screening hypothesis. This work, together with the existing library of over 100 mitochondria-targeting conjugates, lead us to new insights in terms of SAR, and represents a valuable addition to the body of knowledge on the principles governing mitochondrial targeting and its relationship to the emergent biological activity of MTM–small molecule conjugates.

Keywords: mitochondria-targeting, drug discovery, rational design, structural analysis, SAR

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Chemometrically Enhanced Infrared Spectroscopy for Advancing the Biomedical Research on Diabetes Mellitus

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Our research aims at leveraging the molecular sensitivity and specificity of Fourier transform infrared (FTIR) spectroscopy, complemented by chemometrics, to investigate the diabetes-induced alterations in the macromolecular composition of skeletal muscle from diabetic and non-diabetic male individuals.

Skeletal muscles play a key role in carbohydrate, protein and lipid metabolism. They handle about 80% of insulin-driven glucose uptake, making them highly susceptible to metabolic disorders, including diabetes. Understanding how diabetes alters their macromolecular makeup is crucial for a deeper understanding of the molecular background of diabetic myopathies.

Traditional molecular and histochemical assays for analysing tissue composition have some inherent limitations, which we aim to overcome with our proposed approach of chemometrically enhanced FTIR spectroscopy. By applying a multi-stage spectral decomposition of the experimentally obtained FTIR spectra using Multivariate Curve Resolution - Alternating Least Squares (MCR-ALS) approach, we were able to decompose them into several distinct components, with each component representing a certain group of macromolecules. This post-processing approach enabled us to capture a comprehensive biochemical profile of the tissue and establish a set of parameters for the comparison of diabetic and non-diabetic muscles in terms of lipid content, protein secondary structures, collagen, specific amino acids, glycogen, nucleic acids, and other molecular species.

Our approach allows for the simultaneous investigation of numerous macromolecular indicators from a single tissue sample analysed in a single FTIR experiment [1][2], which is essential for understanding disease-related biochemical alteration in tissue and their interrelationships. It provides an efficient methodological framework that is not limited to diabetes-related biochemical changes in skeletal muscle, but can also be applied to other tissues and diseases. These advantages surpass the analytical capabilities of traditional molecular and histochemical tests and emphasise the potential of vibrational spectroscopy to advance biomedical research into diseases.

Keywords: infrared spectroscopy, chemometrics, skeletal muscle, diabetes mellitus, biochemical composition

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The simple Rose water model as a model system for the development of analytical statistical-mechanical models and machine learning approaches

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Recently, the development of water models has focussed on creating more complex models that accurately describe the properties of water molecules. Thanks to advances in computer technology, the use of computationally demanding water models (even ab initio models) is becoming increasingly accessible. However, such complex models are still too computationally expensive for large systems or a wide range of conditions and therefore require too much computational time. Therefore, it is important to develop shortcuts for computationally expensive calculations.

A simple rose water model can be used to develop such shortcuts. The model is two-dimensional and consists of Lennard-Jones discs and an explicit hydrogen bonding potential between them. Due to its simplicity and two-dimensionality, the use of such a model is easier and more intuitive when developing various theories and computational approaches. Here we present how rose water model can be used as a model system for the development of an analytical statistical-mechanical model of water and for the development of a machine learning approach to determine the phase diagram. We have developed a semi-analytical water model that can be used to calculate the structural, thermodynamic and dynamic properties of water in a fraction of the computational time required for simulations [1]. The analytical model is based on the calculation of the probability for each type of interaction and the subsequent generation of snowflake-like structures as an approximation of the structure of liquid water. The accuracy of the analytical model is comparable to standard computer simulations, as the model provides results that are in good agreement with simulations of rose water model. Most of the methods used for the determination of phase diagrams are relatively time consuming.

The computational efficiency of rose water model allowed us to investigate a wide range of conditions and calculate different properties of water throughout the phase space. We have developed an approach that uses unsupervised machine learning algorithms to determine the phase diagram of water, where various simulation data can be used as input to the algorithm [2]. This approach allows an almost automatic determination of the phase diagram based on standard computer simulation data. Two data sets were used to determine the phase diagram. One consists of angular distribution functions, the other of various structural, thermodynamic and dynamic properties.

Keywords: water model, analytical model, phase diagram, unsupervised machine learning

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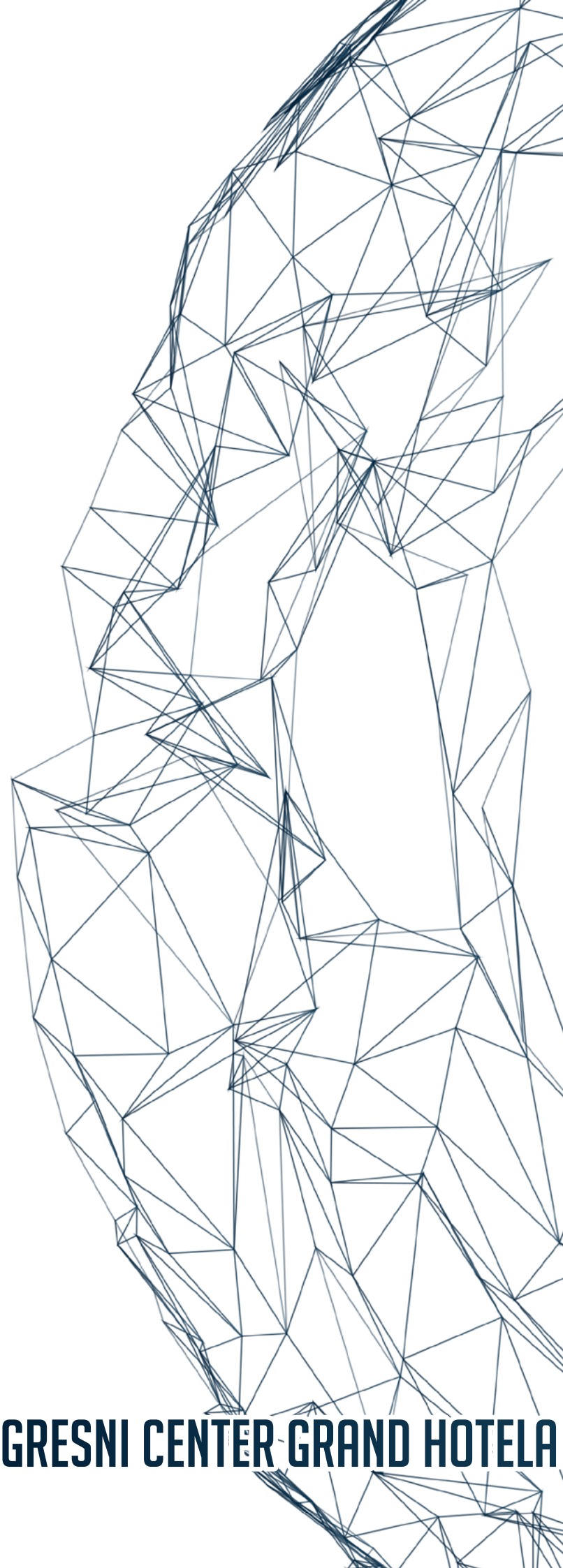

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POSTER PRESENTATIONS

BERNARDIN, PORTOROŽ

Investigating NLP Cytolysin Dynamics: Simulation of Pore Formation in Plant Plasma Membrane

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Global food security is constantly threatened by plant pathogens that cause crop diseases, largely due to the pathogens' ability to develop new invasion strategies through effective co-evolution with their hosts. Microbial plant pathogens secrete a variety of effector proteins to facilitate infection, among which the Necrosis- and ethylene-inducing peptide 1 (Nep1)–like proteins (NLPs) form a significant family. These proteins, produced by bacteria, fungi, and oomycetes, infect a wide range of essential crops, including potatoes, tomatoes, soybeans, grapevines, and tobacco (1).

NLPs are unique cytolytic pathogen effectors known for their ability to permeabilize the plasma membranes of eudicot plants by forming transient small pores. Recently, glycosylinositol phosphorylceramides (GIPCs), major components of plant membranes, have been identified as the binding targets of NLPs on plant plasma membranes. While it is known that NLPs can oligomerize on plant membranes, the precise molecular mechanism of their oligomerization and pore formation remains unclear (2).

This research aims to deepen our understanding of the interaction between NLP toxins and plant plasma membranes. Specifically, we seek to unravel the molecular mechanism behind membrane pore formation induced by NLP monomers and oligomers, as well as the behavior of protein/lipid complexes during membrane attachment. To achieve this, we used AI-based modeling tools and all-atom computer simulations. These methods complement experimental approaches by allowing for the detailed examination of key interactions at the atomic level and the time-dependent observation of the conformational space accessible to protein-lipid complexes. Our findings are expected to contribute to the development of innovative and effective strategies for controlling plant diseases caused by NLP-producing pathogens.

Keywords: Plant pathogen, crop disease, Nep1-like proteins, GIPC, MD simulations

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Ion Chromatographic Determination of Carbohydrates in Kombucha with Electrochemical Detection

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Kombucha is a non-alcoholic fermented tea beverage produced via the metabolic activity of a symbiotic culture of bacteria and yeast. The sugar profile of kombucha varies significantly as a function of microbial activity during the fermentation process, as well as various starting sugar compositions. Anion-exchange chromatography with electrochemical detection is a frequently used technique for carbohydrate analysis since it allows for a direct injection of carbohydrate-containing samples without previous derivatization, while relying on the analytes' weak acidity under elution conditions, as well as their electrochemical activity [1,2]. This represents a particular advantage when analysing food samples, where the matrices are generally complex, and carbohydrates co-exist with organic acids, proteins, and other compounds [3].

In this study, ion chromatography method with electrochemical detection (IC-ECD) was developed and utilized to determine the concentrations of sucrose, glucose, and fructose in kombucha sampled at different fermentation stages (0 – 12 days). The fermentation was carried out at two different ambient temperatures and different starting sugar compositions. Chromatographic separation was achieved using KOH as eluent at 1.0 mL/min flow rate in a 10-minute runtime. Calibration curves in the range of 0.5–15 mg/L for all three analytes yielded consistent retention times and high linearity ($R^2 \geq 0.999$). Kombucha samples were analyzed after controlled unfreezing, filtering, and dilution, whereas the reproducibility was ensured by repeated injections of multistandard solutions. As expected, glucose concentrations consistently decreased over fermentation time, from 45.9 g/L on day 0 to less than 0.1 g/L by day 12. Fructose content decreased more gradually, only losing about 20% of initial content over a period of 12 days. The detection was carried out using a disposable gold working electrode and an Ag/AgCl reference electrode, with optimized pulsed amperometric waveform parameters to maintain electrode integrity over an increased period.

The reported method exhibits sensitivity and reproducibility that are aligned with previously established applications of IC-ECD in sugar-rich matrices. Similar techniques have been used to determine carbohydrate profiles in raw and refined sugar products [1,2], and royal jelly [3]. The present work confirms the suitability of IC-ECD as a powerful analytical tool for fermentation monitoring, and further insight in kombucha and related beverages composition.

Keywords: Ion chromatography; pulsed electrochemical detection; carbohydrates.

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Advanced Electrochemical Sensing of Herbicides: Utilizing Pd-Decorated TiN/Ti_2O_3 Electrodes for Differential Pulse Stripping Voltammetry

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Considering the great importance of water in daily life, the problem of its pollution occupies an important task that must be solved. This results summaries the results of voltammetry studies on the dicamba - 3,6-Dichloro-2-methoxybenzoic acid (DIC) and 2,4-D-dichlorophenoxyacetic acid (2,4-D) using a Pd TiN/Ti_2O_3-GC which are highly polar [1]. Voltammetry analyses have shown that Pd TiN/Ti_2O_3-GC possess superior electrocatalytic activity in contrast to commercial glassy carbon electrode for the red-ox reactions of $K_4[Fe(CN)_6]$. The effect of pH on the electrochemical behaviour of DIC and 2,4-D was investigated in Britton-Robinson buffer solutions (pH 2.0 - 6.0). As found out, the actual pH had a significant influence upon the overall signal-to-noise characteristics, giving to the Pd TiN/Ti_2O_3-GC the best analytical performance at pH 2.0. The oxidation peak of DIC appeared at +0.9 V and 2,4-D at +1.3 V vs. SCE. The experimental conditions optimized for the determination of DIC and 2,4-D in the differential pulse stripping voltammetry mode (DPSV) were: initial potential -0.1 V, end potential +1.7 V, accumulation potential -0.25 V, accumulation time 80 s, and the scan rate 50 mV s^{-1}. The method developed offers linearity in concentration range 4.99 – 53.82 ng/mL, with r = 0.998 for DIC and r = 0.990 for 2,4-D and the limit of detections of 3.03 ng/mL. These results are in the same range with HPLC/DAD, which is used as comparative method. Recovery for DIC and 2,4-D determination in the real sample of river water was 101% for both pesticides.

Keywords: dicamba, 2,4-D, differential pulse stripping voltammetry, pesticides, water

Acknowledgements

This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract number: 451-03-66/2024-03/200017 (J. Milićević and A. Dimitrijević); 451-03-65/2024-03/200124 and 451-03-66/2024-03/200124 (M. Ranđelović)).

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A Vibrational Spectroscopic Approach to Analysing the Organic and Inorganic Matrix of Bone

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Investigating bones – a complex, heterogeneous composite material – through diverse analytical approaches is essential for understanding their structural, functional, and chemical properties within the skeletal system. This is particularly important in archaeological and forensic contexts, where bones are affected by various environmental and post-depositional factors, including acidic soil, heat exposure, moisture, mechanical stress, microbial activity, and pH fluctuations.

Recently, study by Legan et al. have demonstrated the potential of non-invasive reflection FTIR spectroscopy for assessing thermal degradation processes in archaeological bone. [1] The same research group also examined chemical alterations in bone using Attenuated Total Reflectance infrared spectroscopy (ATR) and density measurements obtained through the seldom-used technique of Multidetector Computed Tomography. [2]

The present work explores the application of vibrational spectroscopy in bone analysis, with a focus on various FTIR modalities–including reflection, transmission, and ATR–as well as FTIR imaging and mapping of selected bone samples. Additionally, Raman spectroscopy is employed to complement and compare the FTIR results, offering a broader spectral perspective. Initial analyses were conducted on fresh, defleshed bovine femur bones, which were transversely sectioned to expose all major components of bone structure, including marrow, spongy bone, compact bone, and periosteum. This experimental setup enabled detailed spectroscopic investigation of each region. The insights gained from these controlled experiments will be applied to the study of archaeological bone from various Slovenian archaeological sites, contributing to a deeper understanding of their preservation and historical context.

Keywords: bones, FTIR spectroscopy, Raman spectroscopy, FTIR and Raman imaging, archaeological bones

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Acknowledgement
This work was supported by the Slovenian Research Agency (ARIS) through research project "Next generation analytical tools for heritage science" (J7-50226).

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Development of disposable electrochemical biosensor for organic content detection in marine environment

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Given the escalating threats posed by marine pollution, including devastating oil spills like Deepwater Horizon, [1] there is an urgent need for rapid, sensitive, and deployable sensing technologies to monitor organic pollutants and facilitate timely intervention. Carbon paste-based electrochemical biosensors address this critical gap in environmental monitoring, offering early detection capabilities that could significantly mitigate ecological damage and economic losses associated with such incidents. [2]

The presented work introduces carbon paste-based electrochemical biosensors tailored for marine environments, offering a robust, cost-effective, and user-friendly alternative for on-site determination of organic content in seawater. Using modern additive manufacturing techniques, we developed a disposable two electrode system that utilizes carbon paste electrodes and can detect adsorption of organic content via different voltammetry techniques. The sensing unit is built in a way, that enables it to be submerged, with the electrolyte being simply unmodified seawater. These biosensors leverage the unique advantages of carbon paste electrodes, namely their low background current, wide potential window, and ease of modification, to integrate various biorecognition elements specific to target organic compounds prevalent in marine settings. Fabrication process, operational principles, and analytical performance of constructed biosensors will be shown, highlighting their applicability through both simulated laboratory conditions, as well as tests in marine environment in submerged conditions.

Presented work will cover development and utilisation of biosensor module, that can be attached to a shore-based or buoy-based analytical system and its possibility to be carried by the diver in open waters, offering possibility for early detection of organic sources and possible pollutants and thus giving fast, non-specific indication that possible contaminants are present.

Keywords: electrochemical biosensor, carbon paste, 3D printing, marine environment, organic pollutants

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Contrasting Agents and Methods for Fe^{3+}, Cu^{2+} and H^{+} in SEM/EDS Analysis and 3D X-Ray Tomography

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Bio-based materials such as wood, paper and parchment are often found in important cultural heritage objects. These materials are prone to degradation processes influenced by humidity, temperature and by various ions present. Fe^{3+}, Cu^{2+} and H^{+} (acidity) are known accelerate degradation rates [1]. The main sources of these ions are iron-gall inks, certain pigments as well as contact with different materials containing these elements.

Scanning Electron Microscopy with Energy-Dispersive X-ray Spectroscopy (SEM/EDS) is used to qualitatively and quantitatively determine elements on the surface of the samples within certain atomic mass and concentration limits. The contrast in 3D X-ray tomography strongly depends on atomic mass, enabling three-dimensional visualization of heavier elements, but it cannot distinguish between different elements. Contrasting agents selective to particular ions can enhance detection limits in SEM/EDS analysis and 3D X-ray tomography and can further enable distinguishing between different elements in 3D X-ray tomography. Contrasting agents are compounds containing heavy elements that increase X-Ray absorption coefficient. Ligands with high affinity to specific ions are important in various fields and have been extensively studied [2].

Several ligands were synthesized by introducing heavy elements into structure of specific ligands. These ligands were used as contrasting agents. Both gas phase and solvent based contrasting methods were developed to enhance contrast and detection limit of Fe^{3+}, Cu^{2+} and H^{+} ions in paper and parchment substrates for SEM/EDS analysis and 3D X-ray tomography. Selectivity in the presence of different ions was also evaluated.

The financial support received from the Slovenian Research Agency (ARIS) for programs J7-50226 – NextGenHS, I0-0032 and P2-0273.

Keywords: Contrasting agents, ligands, cultural heritage

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Iridium Catalysis on Polystyrene Support for Hydrogen/Deuterium Exchange

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The synthesis of deuterium-labeled organic compounds typically follows two principal strategies. One involves indirect methods, such as total synthesis using deuterated substrates or reagents. The other employs direct techniques, including hydrogen/deuterium (H/D) exchange or deutero-defunctionalization within the target molecule. Among these, direct H/D exchange is often more efficient and cost-effective, particularly when introducing deuterium into complex molecules like pharmaceutical compounds [1,2].

In both direct and indirect methods, catalysts based on precious metals are commonly employed, with iridium being among the most prevalent due to its high activity in hydrogen isotope exchange reactions [2]. However, homogeneous iridium catalysts pose challenges in recovery and reuse, as they are difficult to separate from reaction mixtures and can deactivate through aggregation.

Immobilizing homogeneous catalysts onto solid supports (e.g., polymers or silica) offers a sustainable approach to catalysis by enhancing recyclability and simplifying purification [3]. This strategy tackles challenges like catalyst recovery, aggregation, and deactivation. Immobilized catalysts are easily separated, often by filtration, and reused with minimal activity loss, reducing precious metal use and aligning with green chemistry principles. It also limits leaching and product contamination, crucial in pharmaceutical synthesis, while combining the performance of homogeneous catalysts with the practicality of heterogeneous ones [4].

With this in mind, we are exploring strategies to develop immobilized catalysts for the synthesis of deuterium-labeled organic compounds, building on established catalytic systems. In this presentation, we will demonstrate the immobilization of a Kerr-type Iridium(I) catalyst onto polystyrene beads. The resulting heterogeneous catalyst was employed in the deuteration of a range of substrates previously investigated using the corresponding homogeneous counterpart. We will discuss the comparative performance of the homogeneous and heterogeneous systems, including recyclability and overall potential for practical applications.

Keywords: H/D exchange, deuteration, immobilization, iridium, catalysis

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Anticancer Potential of Dendritic Poly (aryl ether)-Substituted Polypyridyl Ligand-Based Ruthenium (II) Complexes

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The anticancer activity of ruthenium (II) complexes can be enhanced by incorporating the amphiphilic ligands that possess higher solubility, cellular intake, and targeted drug delivery in comparison to other complexes. Ruthenium (II) complexes of amphiphilic poly (aryl ether) dendrimer based bipyridine ligands were prepared [1] and their anticancer activity was evaluated against three cancer cell lines (A549 lung adenocarcinoma cell line, MDA MB 231 human breast epithelial adenocarcinoma cell lines, and HepG2 liver cancer cell) (**Figure 1**). The selectivity indices of complexes against the cancer cell lines infers that lower generation complexes exhibits consistent and greater selectivity across all the three cell lines, while higher generation complexes show notable potency against HepG2 cells, suggesting its potential for liver cancer treatment. Fluorescence staining assays, AO−EB, DAPI, cell death analysis by PI staining, reactive oxygen species (ROS), mitochondrial membrane potential (MMP) assays and DNA ladder assay were performed for the complexes to understand the anticancer mechanism. The results indicates that these complexes, induces apoptosis in cancer cells through action of DNA and ROS-mediated mitochondrial dysfunction pathways. Molecular docking analysis with DNA and anti-apoptotic Bcl-2 protein supports the experimental observations [2].

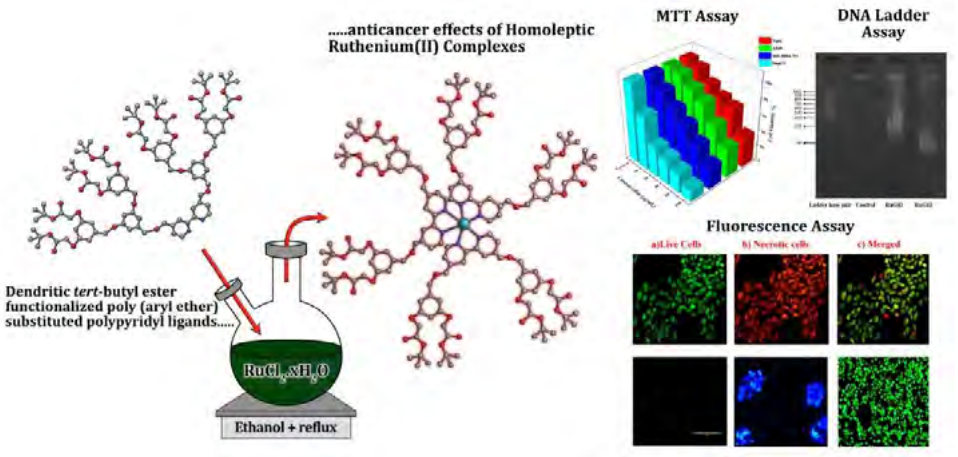

Figure 1. Anticancer studies of Ruthenium (II) complexes of Poly (aryl ether)-substituted polypyridyl ligands.

Keywords: ruthenium complexes, dendrimers, anticancer, *in vitro* cytotoxicity, molecular docking

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Dimethoxy Derivatives of Salicylaldehyde Benzoylhydrazone with Anticancer Activity and Selectivity

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Cancer remains a formidable challenge in modern medicine, characterized by uncontrolled cell growth, invasion into surrounding tissues, and potential metastasis to distant organs. Recent advances in cancer research have greatly expanded the understanding of cancer pathways, resulting creation of new diagnostic and treatment techniques. Small molecules remain the backbone of cancer therapy, even as immunotherapies increase in prevalence. Over recent years, our research has centered on investigating the anticancer properties of hydrazones resulting from salicylaldehyde derivatives and acyl hydrazides. The introduction of a methoxy group in the salicylaldehyde structure has led to derivatives exhibiting potent antiproliferative effects. 3-, 4- and 5-methoxysalicylaldehyde hydrazones demonstrated notable anticancer activity and exclusive selectivity [1-3]. This study further investigates the methoxy substituents within the salicylaldehyde benzoylhydrazone scaffold.

In order to evaluate the anticancer potential of dimethoxy hydrazones and the effect of the position of the methoxy group, a series of five dimethoxy derivatives with different positions of the methoxy groups was designed and synthesized. The compounds were obtained in high yields, and their structures were confirmed by elemental analysis and various spectral techniques.

The compounds were *in vitro* evaluated against a panel of malignant human cell lines of different tissue origin. Dimethoxy hydrazones demonstrated potent activity against the leukemic cell lines at low micro- and nanomolar concentrations. Remarkably, two dimethoxy analogs showed exceptional antileukemic selectivity, with no toxicity observed in normal human embryonic kidney HEK-293 cells. *In silico* modeling elucidated the interaction with the probable target human cAbl kinase, shedding light on the possible mechanism of antileukemic activity of the compounds.

Keywords: salicylaldehyde; hydrazones; methoxy group; antileukemic activity; selectivity

Acknowledgment: The research in this study was funded by the European Union NextGenerationEU, through the National Plan for Recovery and Sustainability of the Republic of Bulgaria, project No. BG-RRP-2.004-0004-C01.

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Synthesis and Bioactivity Evaluation of Cinnamaldehyde Hydrazones

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Cinnamaldehyde, a natural flavonoid, is the compound responsible for cinnamon's distinctive flavor and scent. It belongs to a group of biologically active substances known for a wide array of pharmacological effects, including anti-inflammatory, antibacterial, antioxidant, antimicrobial, and neuroprotective actions [1]. In addition to its ability to inhibit bacterial and fungal growth, cinnamaldehyde shows strong potential as an anticancer agent. Numerous laboratory and animal studies support its capacity to hinder cell proliferation, trigger apoptosis, and arrest the cell cycle [2,3].

This study explores the synthesis, structural characterization, and biological evaluation of new hydrazone derivatives of cinnamaldehyde, formed by combining it with various acylhydrazides. The hydrazides selected incorporate molecular fragments essential for the structure and function of numerous biological compounds. Chemical composition of these cinnamaldehyde-derived hydrazones was established through elemental analysis and mass spectrometry, while IR and NMR spectroscopy confirmed the formation of the hydrazone linkage.

The core biomolecular properties of the cinnamaldehyde hydrazones were predicted using computational modeling via the group contribution method. The compounds exhibit molecular flexibility and optimal lipophilicity, indicating favorable permeability through cellular membranes. Bioactivity profiling suggests that these compounds may interact with GPCR ligands, ion channels, kinases, proteases, and other enzyme systems. Their cytotoxic effects were tested through the MTT assay, revealing that they produce dose-dependent cell toxicity even at low micromolar concentrations.

Keywords: hydrazones, cinnamaldehyde, biomolecular properties, lipophilicity, cytotoxic activity.

Acknowledgment: The research in this study was funded by the Medical Science Council (SMN) at MU-Sofia under Grant No.147/29.05.2024, Project No. 8260/27.11.2023.

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Targeting Amyloid β Aggregates with FDDNP Analogues

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Early and accurate detection of amyloid β (Aβ) aggregates is critical for diagnosing and monitoring Alzheimer's disease (AD). Building on the established FDDNP scaffold, we synthesized and characterized a library of 21 novel analogues designed to improve photophysical properties and Aβ binding performance (**Figure 1**). These compounds were evaluated across various solvents for fluorescence characteristics such as Stokes shifts, quantum yields, and fluorescence enhancement upon binding to $A\beta_{1-42}$ fibrils. Several analogues demonstrated significant improvements, including large Stokes shifts and strong fluorescence turn-on effects, enabling clearer detection in biological environments. Binding affinities were assessed via *in vitro* assays, while selectivity and localization were confirmed in cell-based systems and *postmortem* AD brain tissue. Computational studies – including molecular docking, molecular dynamics simulations, and density functional theory (DFT) calculations – provided insight into binding modes and photophysical mechanisms. This work highlights the potential of tailored FDDNP derivatives as sensitive and selective probes for Aβ detection [1].

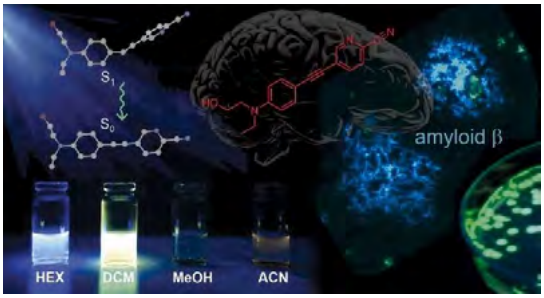

Figure 1: Photophysical and biological evaluation of FDDNP analogues.

Keywords: Alzheimer's disease, amyloid β, synthesis, fluorescent probes.

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Copper-catalyzed light-induced synthesis of β-lactam sulfonamides and divinyl sulfones

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The scope of sulfonyl-containing compounds that can be synthesized has been significantly improved by photoredox catalysis, although the high price and low abundancy of routinely used complexes of ruthenium and iridium has continually driven the development of alternative catalyst, among which copper complexes have attracted significant attention, as they enable access to unique reaction products via the proposed inner-sphere reaction mechanism (ISET). [1]

Copper complexes have been used to promote unique transformations among photoinduced reactions. Among those, we have developed a method to synthesize trifluoromethylated divinyl sulfones from simple alkynes. Reaction takes place by a two-step ATRA (atom transfer radical addition) reaction (Figure 1, a). [2] We have shown that copper complexes were the only ones to enable such transformation among the tested catalysts.

We also prepared a series of sulfonamides containing a β-lactam ring from olefins, utilizing a copper complex as the photoredox catalyst (Figure 1, b). [3] Due to their structural resemblance to existing β-lactam antibotics, they will be tested for potential antimicrobial effect.

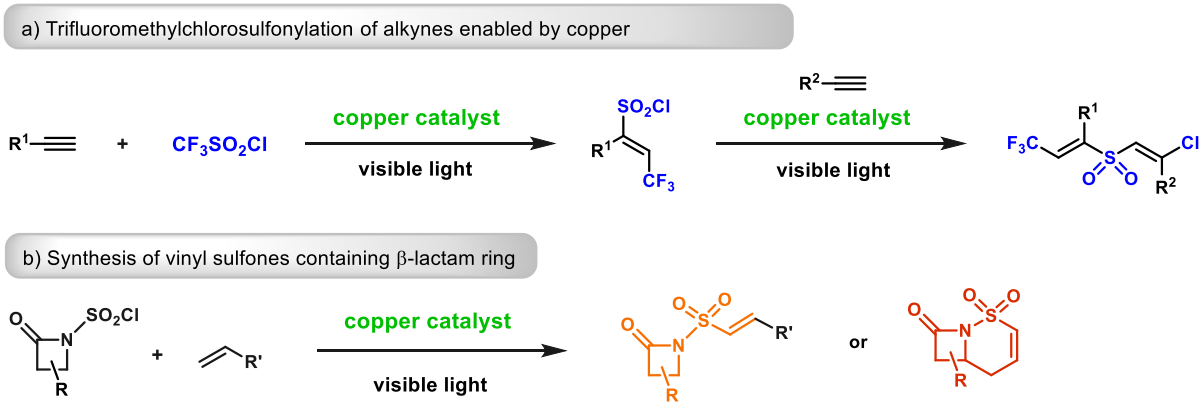

Figure 1: Photoredox-catalyzed synthesis of divinyl sulfones and β-lactam-based sulfonamides.

Keywords: copper complexes, photoredox catalysis, photochemistry, β-lactams, sulfones

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Morphology development in $TiO(OH)_2 \cdot xH_2O$ systems during calcination using different additives

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Nano-scale titanium oxide (nano-TiO_2) are key elements of a wide variety of sectors of advanced materials, devices, and systems in view of their versatility and extraordinary characteristics, mainly optical, electrical and catalytic properties. Thus, nano-TiO_2 is suitable for industry dealing with coatings, papers, inks, toothpaste, pharmaceuticals, plastics, food products, cosmetics, textiles as well as medicine and photocatalysis [1]. TiO_2 exists in different crystallographic structures anatase, rutile and brookite. However, in semiconductor and photocatalytic applications most often anatase TiO_2 structure is used mostly due to its electronic, structural, and surface advantages over rutile [2]. Properties and applications of nanostructured TiO_2 are in turn influenced by synthesis methods, which can be in general divided into two categories: i) TiO_2 synthesis from the liquid phase and ii) TiO_2 synthesis from the vapor phase. On industrial level TiO_2 is still mostly prepared via liquid phase route – sulphate process, in which one of the critical steps is calcination of the crucial intermediate metatitanic acid $TiO(OH)_2 \cdot xH_2O$ into final TiO_2 nanoparticles. Namely, many before mentioned key properties of TiO_2 nanoparticles including crystal structure, crystallite size and surface properties are somewhat affected by the calcination parameters. Therefore, proper kinetic description and morphological development of the system are key to the preparation of TiO_2 nanoparticles with the desired properties.

In this report, we describe the development of morphological characteristics of TiO_2 nanoparticles during calcination in $TiO(OH)_2 \cdot xH_2O$ systems with various additives. Three samples of $TiO(OH)_2 \cdot xH_2O$ (denoted as CCR 150, CCR 200 N and CCR 220 Mn) were obtained from the industrial production of TiO_2 via sulphate process, before the calcination. Sample CCR 150 was pure metatitanic acid $TiO(OH)_2 \cdot xH_2O$ with anatase crystallization seeds, while samples CCR 200 N and CCR 220 Mn additionally contained remains of HCl as acidifying reagent during metatitanic acid hydrolysis (70 g/L and 90 g/L, respectively). Samples were analysed by TG and DTG, coupled with mass spectrometry, as well as SEM, XRD and HTXRD methods. The Rietveld method was used to obtain the phase content data in order to calculate the conversion, needed for the kinetic analysis of a phase transformation. The Avrami method and the linearisation method were used for kinetic calculations.

Morphological analysis revealed that HCl addition during metatitanic acid hydrolysis in general reduces the average size of final TiO_2 nanoparticles from 36 nm to 23 nm and 26 nm in samples CCR 150, CCR 200 N and CCR 220 Mn, respectively. Additionally, an apparent activation energy for $TiO(OH)_2 \cdot xH_2O$ to TiO_2 phase transition was also reduced from 315 kJ/mol to 255 kJ/mol or 205 kJ/mol in the case of samples CCR 150, CCR 200 N and CCR 220 Mn, respectively.

Key words: nano-TiO_2, $TiO(OH)_2 \cdot xH_2O$ calcination, kinetic analysis, morphology development

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Hidrotermalna sinteza in karakterizacija kovinsko-organskih poroznih materialov

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Povzetek

Zaradi vse večjih zahtev po naprednih materialih za energetske in okoljske aplikacije se povečuje zanimanje za kovinsko-organske materiale (*angl. Metal Organic Framework - MOF*). Gre za porozne kristalinične spojine, sestavljene iz kovinskih ionov in organskih ligandov, ki izstopajo po izjemni specifični površini in modularnosti. Ena najpogostejših metod njihove priprave je hidrotermalna sinteza, ki omogoča natančen nadzor nad velikostjo por in strukturo, kar je ključno za prilagajanje njihovih lastnosti specifičnim potrebam. [1] V primerjavi z drugimi metodami hidrotermalna sinteza ponuja boljšo ponovljivost, homogenost vzorcev in je pogosto manj zahtevna iz vidika vzdrževanja ustrezne temperature in tlaka reakcije, čeprav jo lahko omejuje daljši reakcijski čas [2]. Nedavne raziskave spodbujajo nove ter inovativne pristope pri sintezi MOF, kot sta uporaba sinergistično modulirane hidrotermalne metode in uporaba recikliranih surovin, s katerimi je moč doseči višjo stabilnost MOF, izboljšane elektrokemijske lastnosti ter trajnostno sintezo MOF. Ključnega pomena pri sintezi MOF je ustrezna izbira osnovnih gradnikov in sinteznih pogojev, saj ti neposredno vplivajo na strukturne in funkcionalne lastnosti materiala. Različne kombinacije kovinskih ionov in organskih ligandov omogočajo oblikovanje MOF z različnimi stopnjami poroznosti in različnimi adsorpcijskimi kapacitetami, kar je ključno za njihovo kasnejšo uporabo [3]. Pri hidrotermalni sintezi igra MOF zelo pomembno vlogo tudi vrsta uporabljenega topila in njegove lastnosti [2].
V tej raziskavi smo za sintezo kovinsko-organskih ogrodij (MOF) izbrali železov (III) klorid kot vir kovinskih ionov ter tereftalno kislino kot organski ligand. Sinteza je bila izvedena v hidrotermalnem reaktorju, pri čemer smo kot topilo uporabili mešanico vode in etanola. Pri izbranem razmerju surovin smo preučili vpliv različnih reakcijskih pogojev (temperature in reakcijskega časa) na oblikovanje ter kakovost nastalih MOF. Pridobljene produkte smo karakterizirali z metodami kot so elektronska mikroskopija, rentgenska praškovna difrakcija, FTIR analiza, BET analiza specifične površine in velikosti por materiala ter temperaturno programirano desorpcijo. Preučili smo tudi termično stabilnost MOF in določili porazdelitev velikosti delcev. Dodatno smo preučili vpliv dodatka globoko evtektičnega topila na sintezo MOF ter njihove kemijske lastnosti. Rezultati kažejo, da že pri relativno nizki temperaturi in kratkem času sinteze dobimo MOF z obetavnimi lastnostmi, kar kaže na učinkovitost hidrotermalne sinteze tudi pri zmernih pogojih.

Ključne besede: kovinsko-organska ogrodja, reakcijski pogoji, železov (III) klorid, tereftalna kislina, globoko evtektično topilo, hidrotermalna sinteza

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Tailoring the morphological properties of ZIF-94 by binary solvent mixtures

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Zeolitic imidazolate frameworks (ZIFs), a subgroup of metal-organic frameworks (MOFs), have in recent years been extensively studied for sorption applications, also CO_2, due to their superior stability and kinetics for vapour/gas adsorption if compared to carboxylate-based MOFs. The ZIF-94 (alternative name is SIM-1) is a well-known and studied ZIF with potential uses in CO_2 capture (2.2 mmol @25°C 1bar) and CO_2/N_2 separation when used as part of Mixed Matrix Membranes. One of the problems with utilising ZIF-94 in sorption and separation applications is that, like some other ZIF frameworks, the flexibility of the metal coordination means that some linker and metal combinations in the synthesis mixture often lead to multiple stable phases with different topologies, including ZIF-93/94 system with 5-methyl-imidazole-4-carbaldehyde as a linker and ZIF-71/72 synstem with 4,5,-dichloroimidazole as a linker. The two co-existing phases in such systems show either vastly different porosity (ZIF-71/72) or a significant change in gas isotherm shape and final gas/vapour uptake (ZIF-93/94). In this context, a crucial problem when trying to optimise the reported ZIF-94 synthesis is that often mix phase systems form.

We are reporting here on a successfull preparation of phase pure ZIF-94, both mechanochemically and solvothermally, using only ethanol and water as solvents. The synergistic use of ethanol's structure directing role and water as a kinetic modifier allowed for preparation of well crystalline ZIF-94 with clearly defined cubic particles. The use of ethanol/water instead of more common THF also allowed for easier activation of the resulting ZIF, reducing the required solvent needed for washing and solvent-exchange, thus making the synthesis ever greener. Variation in solvent composition and temperature, allowed us to have morphological control over particle size and to some extent shape. Only at very high water compositions, the ZIF-93 was observed.

Keywords: Zeolitic imidazolate frameworks, metal-organic frameworks, green synthesis, morphology control

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Structural and magnetic characteristics of Fe_3O_4/ZIF-8 as nanoadsorbent for potential environmental applications

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With the rapid advancement of industrialization, the discharge of industrial waste has emerged as a significant global water pollution issue. Among the various contaminants found in water, heavy metal ions are the most prevalent, frequently detected in water systems, posing serious risks to human health. As a result, numerous effective strategies and technologies have been employed to detect and remove these pollutants, including adsorption onto various nanoadsorbents. Chemical adsorption is widely utilized in water purification due to its cost-effectiveness and low energy requirements. Consequently, the development of highly efficient and selective nanoadsorbents for removing toxic pollutants significantly increased research attention and has become a primary focus in the field of adsorption science. Metal–organic frameworks (MOFs), also referred to as porous coordination polymers, are crystalline microporous materials constructed from metal ions or clusters connected by organic linkers. These innovative nanomaterials have attracted significant attention due to their large surface area, customizable structures, and controllable pore sizes [1,2].

Nanoadsorbent Fe_3O_4/ZIF-8 was synthesized as follows, both zinc acetate (ZnAc) and 2-methylimidazole (2-MIM) were dissolved in water. Magnetic nanoparticles (MNPs) were prepared in a water solution with three different concentrations (10 mg/mL (10/Fe_3O_4/ZIF-8), 20 mg/mL (20/Fe_3O_4/ZIF-8), 30 mg/mL (30/Fe_3O_4/ZIF-8)), added to the 2-MIM solution and vortexed for 30s. The morphology by SEM confirmed cubic crystal structure of prepared nanoadsorbents, while FTIR analysis confirmed the Zn-N and imidazole C-H vibrational stretching and showed the presence of Fe-O bonds. Such strategies for magnetically derivable nanoadsorbents offer promising ways to facilitate environmental remediation, while displaying excellent reusability and reduced processing costs.

Keywords: metal-organic frameworks, magnetic nanoparticles, ZIF-8, nanoadsorbent

Acknowledgement: This research was supported by the Slovenian Research Agency (ARRS) within the frame of program P2-0046 (Separation Processes and Production Design), program P2-0114 (Applied electromagnetics), project No. L2-4430 (Production, Isolation and Formulation of Health Beneficial Substances from *Helichrysum italicum* for Applications in Cosmetic Industry).

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Processing-property relationships in rapidly sintered microcrystalline Nd-Fe-B permanent magnets

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The fabrication of sintered Nd-Fe-B permanent magnets is traditionally based on powder metallurgy processes involving time-intensive high-temperature sintering. While effective, this conventional route often results in excessive grain growth and limited control over the microstructural evolution, which in turn constrains the achievable magnetic performance. Rapid sintering methods, such as Spark plasma sintering (SPS), present a promising alternative by facilitating densification at lower temperatures and with significantly shortened processing times. Nevertheless, the non-equilibrium nature of SPS introduces distinct challenges related to phase stability and microstructural uniformity.

In this study, we explored the effects of SPS process parameters on the structural and magnetic characteristics of bulk samples prepared from anisotropic, microcrystalline Nd-Fe-B powders. Two primary issues were identified: (i) localized decomposition of the hard-magnetic $Nd_2Fe_{14}B$ phase due to Joule heating at interparticle contacts, and (ii) insufficient formation of the Nd-rich grain boundary phase, partially attributed to residual hydrogen within the powder [1]. Adjustments to the electrical input during consolidation were effective in minimizing phase decomposition and preserving the hard-magnetic phase. Furthermore, implementing a hydrogen degassing step prior to sintering led to a more uniform distribution of the grain boundary phase.

Processing at approximately 880 °C enabled significant grain refinement, achieving a ~33% reduction in grain size compared to conventionally sintered counterparts. This refinement was accompanied by a >15% increase in coercivity and an improvement in the temperature stability of coercivity, with the temperature coefficient decreasing from −0.65 to −0.58%/°C. These results emphasize the capability of SPS to enhance the microstructural and magnetic properties for magnets based on standard Nd-Fe-B powders, provided that critical process variables are carefully managed.

Ključne besede: SPS/FAST, Nd-Fe-B magnets, rapid sintering, microstructure refinement

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A Rapid Consolidation Route for Recycling End-of-Life Nd-Fe-B Magnets by low-energy Radiation Assisted Sintering (RAS)

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Nd-Fe-B permanent magnets are critical components in electric vehicles, wind turbines, and high-efficiency electronics. However, their production is dependent on rare-earth-elements (REEs), which face significant supply risks and environmental burdens. Recycling Nd-Fe-B magnets from end-of-life (EOL) products offers a more sustainable alternative to virgin production, but conventional sintering methods remain energy-intensive and time consuming. While Hydrogen Processing of Magnetic Scrap (HPMS) enables selective extraction of Nd-Fe-B powders, these powders suffer from oxidation and degraded grain boundary phases, reducing the achievable magnetic properties, which cannot be resolved using traditional vacuum sintering.

To overcome these barriers, we investigated Radiation-Assisted Sintering (RAS) as a low-energy, rapid consolidation method for HPMS-derived Nd-Fe-B powders. We evaluated its densification capability, magnetic performance, and response to grain boundary restoration using NdH_3 and TbF_3 additives. This paper reports the magnetic properties, grain size distributions, and energy demands of RAS-processed recycled magnets, benchmarked against conventional sintering. HPMS powders were jet-milled in argon-atmosphere, maintaining a lower oxygen content. Powders consolidated by RAS achieved remanence values equal to or higher than the EOL magnet and coercivities up to 822 kA/m at 100°C, when both additives were applied. RAS supressed grain growth more effectively than conventional sintering, while also reducing the energy consumption by ~90%.

RAS is a viable, energy-efficient alternative to conventional sintering for recycled Nd-Fe-B magnets. It enables property recovery equal to or better than the EOL material, supporting a more circular and sustainable magnet supply chain, showing potential for process scaling, and an integration into the recycling loop.

Keywords: Nd-Fe-B Permanent Magnets; Magnet Recycling; Critical Raw Materials; Sustainability

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Studying degradation of commercial Li-ion cells using low-frequency Electrochemical Impedance Spectroscopy

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Studying degradation in lithium-ion batteries is essential for improving performance, safety, cost, and sustainability. Key mechanisms include solid electrolyte interphase (SEI) growth and lithium plating at the anode, transition metal dissolution and structural changes at the cathode, particle cracking, delamination and electrolyte decomposition and depletion at high voltages or temperatures. These processes lead to capacity fade, increased internal resistance, and in extreme cases even to severe safety risks like thermal runaway. Electrochemical impedance spectroscopy (EIS) is a powerful technique that is particularly useful for degradation studies, as it allows for non-invasive investigation of time resolved processes, distinguishing phenomena such as ohmic resistance, interfacial kinetics and ion diffusion [1,2]. Still, determining which of the degradation processes is the prevailing one in the studied system remains challenging. Both electrodes share the same electrolyte and lithium inventory and changes in one electrode can indirectly affect the behavior of the other, making it difficult to isolate one mechanism from another. In addition, when performing electrochemical measurements on a commercial lithium-ion cell, the observed responses reflect the combined contributions of all cell components, including both electrodes, electrolyte, and electrode configuration.

In this work, high-energy NMC-Graphite(+SiOx) cylindrical commercial battery cells (type 18650) were electrochemically (galvanostatically) cycled under various conditions. Cells were cycled at different temperatures (23°C or 45°C) within various depths of discharge (DoD). State of health (SoH) of a battery was determined by designated capacity measurements and was periodically monitored after specific numbers of cycles. In parallel, EIS measurements down to very low frequencies (0.1 mHz) were performed in order to determine the additional contributions that are not accessible by more conventional frequency ranges e.g. to 10 mHz. A possible approach to separate the contributions from the anode and the cathode is to disassemble commercial cells after cycling and examine each electrode individually. Besides a variety of techniques for assessing the physico-chemical state of the electrodes, electrochemical characterization (particularly EIS) is of critical importance. In the present work, we use a variety of laboratory cell types to electrochemically evaluate degraded electrodes, including half-cells, symmetric cells and 3-electrode cells with a lithiated gold micro-reference electrode. A combination of these cell types allows for a variety of tests and enables us to gain a comprehensive understanding of the electrochemical state of each degraded electrode.

Keywords: Li-ion batteries, degradation, electrochemical impedance spectroscopy, micro reference electrode

Acknowledgments

Lana Regent and Jože Moškon gratefully acknowledge the financial support of the Slovenian Research Agency within the project J2-4463. Robert Dominko gratefully acknowledges the financial support of the Slovenian Research Agency within the national programme No. P2-0423. Miran Gaberšček acknowledges the financial support of the Slovenian Research Agency within the national programme No. P2-0393.

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Anisotropy limitations in additive manufacturing with material extrusion

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In this study, we explore the challenge of creating anisotropic permanent magnets through the process of additive manufacturing, specifically using material extrusion (MEX). Typically, the production of anisotropic magnets requires the application of an external magnetic field, with the most cost-effective approach being the utilization of permanent magnets in a specific orientation to align the particles. However, when employing a filament-based 3D printer or material extruder, generating an adequate magnetic field presents certain difficulties. The simplest method involves printing directly atop a permanent magnet, as shown in previous studies. [1] However, this approach restricts the magnet's height due to the diminishing magnetic field with distance, eventually leading to a point where particle orientation ceases. Contrary to predictions, our observations revealed that the printed magnet not only sustains but also extends the magnetic field of the underlying permanent magnet. This results in a greater degree of anisotropy at distances further from the magnetic field source than initially anticipated. This discovery opens up new possibilities for more intricate designs, circumventing the limitations imposed by space constraints for permanent magnet placement by leveraging the magnetic field extension provided by the previously printed magnet

Keywords: Anisotropic, Additive manufacturing, Material extrusion (MEX), Permanent magnets, Magnetic field extension

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Microwave-assisted Transformation of Insoluble Ammonium Polyphosphate Powder into Soluble Transparent Thin Foil

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Ammonium phosphate compounds are widely used in agriculture as fertilisers (source of nitrogen and phosphorus) and in fire protection as flame retardants (in dry chemical fire extinguishers and composite materials). The most common types, monoammonium phosphate (MAP; $NH_4H_2PO_4$), diammonium phosphate (DAP; $(NH_4)_2HPO_4$), and ammonium polyphosphate (APP; $H(NH_4PO_3)_nOH$), differ in chemical structure, physical form, solubility, and application conditions.

MAP and DAP are crystalline solids (white to off-white crystalline powders or granular material) with high water solubility at ambient conditions. However, APP exists on the market in two main forms: solid (usually as a white powder or granules) and liquid (aqueous solutions). Depending on its polymerisation degree, APP ranges from fully water-soluble (used in liquid fertilisers; contains from 2 to 10 monomers in the chain) to slowly soluble or even insoluble in water (used as a flame retardant in organic-polymer and construction materials; contains more than 100 monomers in the chain). Water-based processing of the less soluble forms requires either elevated temperatures or acidic conditions to facilitate chain breakdown.

However, the highly soluble APP in a frozen intermediate state between powder and liquid, which could be used as a flame-retardant layer on electronic parts, does not exist. Therefore, in this study, the insoluble commercial flame-retardant APP was mixed with water in different mass ratios. The homogenous suspension was applied to a glass plate before it was irradiated with high-power microwaves (1000 W) in an inverter microwave until all water evaporated. Thermal depolymerisation of APP under microwave irradiation transformed white powder into a layer of white film to transparent foil, depending on the mass ratio of APP to water.

Transparent foil kept the flame-retardant properties, however, solubility in water increased. Low-solvent film formation from solid powder was evaluated by FTIR, XRD, SEM and EDXS, TG, IC and ICP-OES, which have all proven chemical and physical changes.

Microwave heating of the aqueous suspension promoted rapid localised temperature rise, which led to partial thermal depolymerisation of the polyphosphate chains. Water acted as both a transient plasticising medium and a heat-transfer agent, which enabled APP to undergo a softening transition, allowing molecular mobility sufficient for film-foil coalescence before complete evaporation of the water, which led to the freezing of the state. This study opened a new field for organic materials in connection with microwave irradiation.

Keywords: ammonium polyphosphate; microwave irradiation; volumetric heating; breaking chemical bonds; thin foil

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Uporaba tankoslojnih premazov za zaščito kovin pred korozijo v kislem mediju

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Korozija kovin v kislih okoljih predstavlja eno izmed osrednjih tehnoloških in gospodarskih težav številnih industrijskih panog, zlasti naftne industrije, kemične predelave in metalurgije. Med najbolj agresivne korozivne medije sodi klorovodikova kislina (HCl), ki se pogosto uporablja pri postopkih čiščenja in jedkanja kovinskih površin ter pri stimulaciji vrtin v naftni in plinski industriji. Zaradi njene izrazite agresivnosti lahko že v kratkem času povzroči znatno degradacijo kovinskih materialov. Zato je razvoj učinkovitih zaščitnih premazov ključnega pomena za podaljševanje življenjske dobe kovinskih komponent ter za zmanjševanje stroškov vzdrževanja in popravil.V predstavljeni raziskavi smo preučevali zaščitne lastnosti tankih filmov na osnovi titanovega dioksida, pripravljenih po sol-gel metodi, v treh različnih koncentracijah raztopin HCl (2.0, 8.5 in 17.0 wt%). Sol-gel metoda je bila izbrana zaradi njene preprostosti, možnosti natančnega nadzora nad kemijsko sestavo in mikrostrukturo nastalega sloja ter zaradi nizkih stroškov priprave. Učinkovitost Ti^{4+} prevleke v 2.0, 8.5 in 17.0 wt% HCl je bila merjena in preučevana z elektrokemijskimi metodami, kot je elektrokemijska impedančna spektroskopija (EIS). Rezultati nakazujejo, da ima Ti^{4+} prevleka učinkovito odpornost in pozitivne lastnosti zaviranja korozije zaradi nanešenih večih tovrstnih slojev, pri čemer je najboljše protikorozijske lastnosti pokazala kovina, zaščitena s petimi sloji sušenimi pri 200 °C ob posamičnem nanosu. Najvišja učinkovitost zaviranja korozije, več kot 99.0 % je bila dosežena, ko je bila zaščitena površina izpostavljena 8.5 wt% HCl za 25 ur, medtem ko je pri 17.0 wt% HCl znašala $\eta = 94$ %, vendar se je z daljšo izpostavljenostjo začela zmanjševati in po 25 urah padla na 64 %. Eksperimentalni rezultati so pokazali, da TiO_2-tanki filmi zagotavljajo učinkovito zaščito. Upad učinkovitosti je mogoče pripisati postopni degradaciji zaščitnega TiO_2-sloja v izjemno agresivnem mediju, kar vodi v zmanjšano zaščito osnovnega kovinskega materiala. V prihodnje bi kazalo nasloviti izboljšanje z dodatnimi površinskimi modifikacijami, dopiranjem TiO_2 ali kombiniranjem z drugimi funkcionalnimi materiali.

Ključne besede: kislinska korozija, AISI 304, Ti^{4+} premazi, EIS

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Raman, SERS and DFT study of selected polyphenols (ellagitannins and gallotannins)

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Polyphenols are natural compounds widely found in plants, with tannins being one of the most abundant classes. This study investigates the vibrational properties of selected ellagitannins and gallotannins and their interactions with metal ions, combining experimental spectroscopy and computational methods to better understand their complex structures. Characterizing polyphenols (tannins) and their metal interactions is important in fields such as medicine, agriculture, pharmaceuticals, and cultural heritage. For example, iron-gall inks (metal-polyphenol complex) were extensively used from the 5th to the 19th century and pose conservation challenges due to their corrosive nature.

Raman spectroscopy offers detailed molecular structural information by analysing inelastic light scattering associated with specific vibrational modes. Surface-Enhanced Raman Spectroscopy (SERS) is based on the amplification of weak Raman signals using nanostructured metallic substrates, enabling sensitive detection at low concentrations. In this work, (FT)-Raman spectra of selected ellagitannins; vescalin, castalin, vescalagin, and castalagin (isolated via preparative liquid chromatography) were recorded using 785 nm and 1064 nm excitation. SERS spectra were collected with citrate-reduced silver colloids at 532 nm excitation. Despite their structural similarities, minor spectral differences were observed and compared with theoretical simulations. Furthermore, iron complexes of these ellagitannins were prepared and analysed to identify metal-binding sites [1] (e.g. changes and shifts in carbonyl (ν(C=O)) vibrational bands). Additionally, Raman and SERS spectra of commercially available tannic acid and its complexes with iron and copper ions were studied. Complementary Density Functional Theory (DFT) calculations simulated vibrational spectra and modelled metal coordination with tannic acid (gallic acid esters of glucose), providing molecular-level insight into polyphenol-metal interactions.

This integrated approach advances understanding of polyphenol (tannin) structures and their metal binding, relevant for biological applications and the preservation of historic iron-gall ink manuscripts.

Keywords: Raman spectroscopy, Surface-Enhanced Raman Spectroscopy, ellagitannins, gallotannins, DFT

Acknowledgment. The authors would like to thank the Slovenian Research and Innovation Agency (ARIS) for the following grants (projects): Z1-4404, J7-50226, P1-0447.

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g-C_3N_4 based materials for solid-state hydrogen storage

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The global shift towards clean and renewable energy sources has intensified research into efficient and safe hydrogen storage systems. Among the various hydrogen storage methods, solid-state storage has gained significant attention due to its potential for high volumetric density, reversibility, and safety under ambient conditions. Materials such as metal hydrides, complex hydrides, and porous frameworks have been extensively studied, but challenges remain in terms of storage capacity, kinetics, and cycling stability [1-4].

Graphitic carbon nitride (g-C_3N_4), a layered polymeric material composed mainly of carbon and nitrogen, has recently emerged as a promising platform for solid-state hydrogen storage. Its high thermal and chemical stability, moderate surface area, and tunable electronic structure make it an ideal candidate to form advanced composite materials [3,4]. They can either be formed with another semiconductor (e.g. TiO_2, $CoMn_2O_4$, etc.) or with impregnation/doping of metals (e.g. Pd, Ni, Pt, Mg etc.) [1-4]. Thus, composite materials offer new design opportunities for lightweight, efficient, and cost-effective hydrogen storage systems.

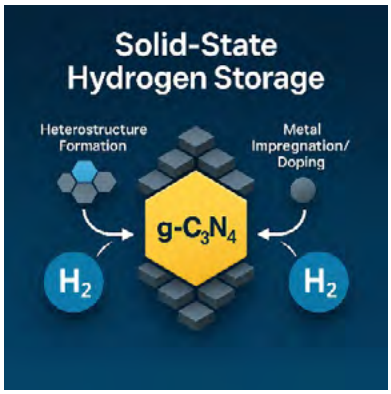

Figure 1. Conceptual diagram of the study.

In this study, we investigated various g-C_3N_4-based materials, either as pure components or composite materials, and studied their potential in solid-state hydrogen storage. The g-C_3N_4 base material was synthesized by calcining 2 g of dicyandiamide in air at 642 °C for 3.33 h, with a heating rate of 225 °C/h [5]. We then employed various strategies, such as heterojunction formation or depositing metals (Fig. 1), to introduce a secondary component aimed at enhancing hydrogen affinity and lowering the temperature required for hydrogen release. Characterization by chemical, surface, and textural sensitive techniques (FTIR, DRIFTS, TGA, XRD, TPD, TPR, etc.) provided insights into the materials' properties, which were preliminarily evaluated for possible solid-state hydrogen storage applications.

Acknowledgement: This research was funded in part by the Austrian Science Fund (FWF) [10.55776/COE5] (Cluster of Excellence MECS).

Keywords: g-C_3N_4 materials, solid-state hydrogen storage, environmental applications, energy storage.

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Cantor entropy-alloys as electrocatalysts for hydrogen-evolution reaction

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Medium- and high-entropy alloys (MEAs and HEAs) are gaining attention as novel electrocatalysts for hydrogen evolution reactions (HERs), due to their compositional flexibility, tunable microstructures, and inherent structural stability. In this study [1], a series of Cantor-based MEAs (CoFeNi, CoFeNiMn, and CoFeNiCr) and a HEA (CoFeNiMnCr) were synthesized using a simple inert-gas arc melting method. The MEAs generally solidified into large grains with single-phase face-centered cubic (FCC) structures and homogenous elemental distribution. In contrast, the HEA displayed finer grains and the presence of secondary phases such as Cr-rich carbides and Mn oxides, both within grains and along grain boundaries. The CoFeNiCr alloy was distinguished by the coexistence of two FCC matrix phases, with one phase notably enriched in Cr. XRD analysis confirmed these phase structures and indicated that the lattice parameters varied slightly with composition, a result attributed to differences in the atomic radii of the constituent elements.

Electrocatalytic performance for HERs was assessed in both alkaline and acidic media using a specially designed electrochemical cell. The alloys demonstrated promising activity when benchmarked against Pt foil. In alkaline media, the overpotential trend followed: CoFeNi < CoFeNiMn ⩽ CoFeNiCr < CoFeNiMnCr. In acidic conditions, the trend was: CoFeNiMn < CoFeNi < CoFeNiMnCr < CoFeNiCr. These trends were linked to the alloys' elemental makeup. In alkaline media, the Co-Fe-Ni combination provided an optimal hydrogen binding affinity (HBA), while in acidic media, performance was influenced by the cumulative effect of all elements. Tafel slope analysis showed similar trends, with lower slopes observed for alloys containing multiple matrix phases, supporting enhanced hydrogen spillover mechanisms. All samples showed high electrochemical stability in alkaline environments. Alloys with Cr, particularly CoFeNiCr and CoFeNiMnCr, also maintained stability in acidic conditions, which is attributed to their corrosion-resistant nature and complex microstructures.

These results emphasize the potential of Cantor-based MEAs and HEAs as efficient and durable electrocatalysts. Their adjustable properties, driven by high-entropy design principles, offer new strategies for developing robust materials tailored for water-splitting applications in clean hydrogen production.

Keywords: Medium-entropy alloy, High-entropy alloy, Water splitting, Hydrogen binding energy, Spillover effect

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Investigation of the synthesis parameters towards uniform-sized PbS quantum dots

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Quantum dots (QDs) are among the most promising materials to meet the requirements for the development of the advanced optoelectronic devices. Some of their favourable properties include solution-processing, substrate compatibility and, most importantly, adjustable bandgap size based on quantum size effect. Lead (II) sulphide (PbS) QDs are one of the prime candidates in wide industrial use due to their highly tuneable optical properties. For this reason, development of PbS QDs with uniform size and good surface passivation is a prerequisite for their use in high-performance optoelectronic devices.[1]

Until now, PbS QDs have been successfully synthesised by different methods, such as: hot injection synthesis, cation exchange, drop/spin coating, etc. One of the most successful, methods for obtaining monodispersed colloidal PbS QDs remains the Hines synthesis which involves the injection of highly active sulphur precursor into a lead-precursor solution.[2] However, a great care must be taken when using this method, as the heating time after injecting the sulphur precursor or even slightest modifications of precursor ratio can lead to QDs with a wide size distribution.

In this work, we examined Hines synthesis in details, in terms of lead and sulphur ratio, type of surfactant, temperature and heating time on the nucleation and growth of PbS QDs. The main methods to characterise the obtained QDs was transmission electron microscopy to determine their size distribution, while their optical properties were assessed by measuring optical absorption and emission.

Keywords: quantum dots, lead (II) sulphide, size-property relations, transmission electron microscopy, optical properties

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Acknowledgement. Authors acknowledge the Slovenian Research Agency for funding through the research core program P2-0089 and the research project GC-0003.

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Utilization of plasmonic effects for the photocatalytic removal of bisphenol A under visible light

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This research focuses on heterogeneous photocatalysis for wastewater treatment, using visible light to activate photocatalysts. Titanium dioxide (TiO_2) is a key material due to its high photocatalytic activity, low toxicity and water stability. However, due to its wide band gap, its activation is limited to UV light [1,2]. To address this limitation, plasmonic metals (PM) such as Au, Ag and Pt were deposited on titanate nanorods (TNR) to enhance visible-light-driven photocatalysis by localized surface plasmon resonance (LSPR). The study also investigates in detail how different PM affect the properties of TNR+PM photocatalysts.

TNR+PM catalysts were prepared using a wet impregnation method, where in-house prepared TNR were stirred in a PM precursor/ethanol solution for 2 hours, followed by calcination at 300 °C in an atmosphere of 5% H_2/95% N_2 with a heating ramp of 150 °C/h [3,4]. The structural and optoelectronic properties of the materials were characterized using various techniques such as UV-Vis DR, solid-state PL, TCSPC, N_2 physisorption, SEM-EDXS, XRD and TEM. The photocatalytic performance of the materials under visible-light illumination was evaluated by measuring the generation of reactive oxygen species (ROS) and the degradation of bisphenol A (BPA), a model organic pollutant.

SEM-EDXS analysis confirmed that the actual PM loading was approximately 1.0 wt.%, which is consistent with nominal values. The TNR+PM samples showed a uniform distribution of PM, with particle sizes varying according to metal type: Pt exhibited the smallest average particle size (1.5 nm), while Au had the largest (45 nm). These differences were influenced by the pH of the PM precursor solutions relative to the isoelectric point of TNR. The addition of PM to TNR resulted in an extended fluorescence lifetime, which improved the catalytic properties. Solid-state photoluminescence (PL) measurements revealed that TNR-Pt had the lowest charge carrier recombination rate among all tested materials. ROS generation tests using various water-soluble target molecules (e.g., DPPH, $ABTS^{\bullet+}$ and coumarin) confirmed that the photocatalysts were able to generate superoxide anion ($O_2^{\bullet-}$) and hydroxyl ($OH^{\bullet}$) radicals under visible light. Additionally, all TNR+PM catalysts tested were shown to generate ROS due to the LSPR effects of the plasmonic metals when illuminated at 550 nm and using coumarin dissolved in water as the target molecule. Among the catalysts, TNR-Au showed the lowest charge carrier generation and BPA degradation rate. In contrast, TNR-Pt with its smallest nanoparticles and the most suitable energy band distribution showed the highest ROS production and BPA degradation efficiency. These results indicate that superoxide anion radicals ($O_2^{\bullet-}$) are the primary drivers of BPA oxidation and degradation on TNR+PM catalysts, with TNR-Pt outperforming the other catalysts due to its enhanced ROS generation and superior photocatalytic activity.

Keywords: heterogeneous photocatalysis, titanium dioxide, plasmonic metals, wastewater treatment

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Improving the Usability of Photocatalytic Water Treatment through Immobilised Thin Films and Reactor Configuration

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The immobilisation of semiconductor photocatalysts is a crucial step towards a scalable and sustainable implementation of heterogeneous photocatalysis in water treatment technologies. Coating photocatalysts on inert solid supports prevents loss of the catalyst during operation and eliminates the need for complex separation processes such as filtration or centrifugation, which are often required for suspended powders [1]. This greatly simplifies the operation of the reactor and improves the long-term reusability and mechanical durability of the photocatalyst. In addition, immobilised configurations are well suited to continuous flow and recirculation reactor systems. They allow precise control of liquid dynamics, light exposure and residence time, factors that are critical for optimising photocatalytic efficiency. Transparent or reflective substrates such as glass also promote uniform light distribution and minimise scattering losses, which improves photon utilisation when irradiating with light [2].

In this study, a thin TiO_2 film was deposited on microscope glass slides by spin-coating from a TiO_2-ethanol-TEOS suspension, followed by thermal treatment to improve adhesion and film stability. The photocatalytic activity was investigated in a specially designed batch-recycle reactor (with a circulation rate of 50 to 200 ml/min) using coumarin (with a molarity of 0.7 to 2.8 mM) as a fluorescent probe for the formation of hydroxyl radicals (˙OH). The formation of 7-hydroxycoumarin (7OH-CUM) was monitored *ex situ* by photoluminescence measurements using a Perkin Elmer LS-55 fluorescence spectrometer. A ScienceTech TLS-55-X300 tunable light source was used to illuminate the catalyst. This allowed us to adjust the wavelength (λ=365 to 550 nm) and the intensity of the light (from 80 to 100%).

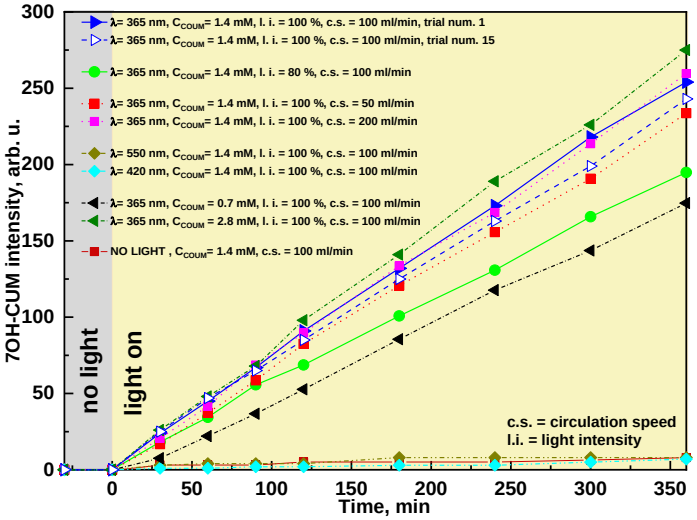

Figure 1. Generation of 7-hydroxycoumarin (7OH-CUM) as a function of reaction time.

The results in Fig. 1 show that ˙OH production is strongly influenced by photon flux, spectral distribution and hydrodynamic conditions, with the highest 7OH-CUM yields observed at 365 nm illumination at full intensity and optimal circulation rates. Control experiments confirmed the photocatalytic nature of the reaction. The TiO_2 film proved to be robust as its photocatalytic activity decreased only slightly even after 15 repeated trials.

These results show that the TiO_2 film immobilised on glass substrates is effective, reusable and robust under the tested operating conditions and that its integration into batch recycling systems for industrial-scale photocatalytic water treatment is promising.

Keywords: TiO_2 photocatalysis, hydroxyl radicals, immobilized catalyst, spin coating, batch-recycle reactor

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Solar-light-driven photocatalytic activity of WO_3 with incorporated titanium for degradation of selected pharmaceuticals

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The ever-increasing occurrence of pharmaceutical residues in water bodies has created major concerns because of their persistence and ecological effects as far as aquatic life is concerned. One of the possible sustainable approaches to the breakdown of these contaminants involves the use of photocatalysis by the semiconducting metal oxides using solar light. The relatively low band gap of tungsten oxide (WO_3) positioned in the visible range (~2.8 eV, λ = 442 nm) [1] makes it a good candidate for photocatalytic degradation of pharmaceuticals under solar light. We present the results of the WO_3 that has been structurally and optoelectronically modified by incorporation of titanium into the tungsten oxide matrix (W/Ti oxide). A set of WO_3 and W/Ti oxide powders has been synthesized by sol-gel method while the titanium concentration was set to 0, 1, 10, and 20 atomic percent [2]. The obtained W/Ti oxide powders have been systematically characterized. XRD analysis confirmed that the crystal symmetry changes gradually from monoclinic (pure WO_3) to tetragonal and finally cubic phase as the concentration of titanium reaches 10 at.%, proving that titanium ions stabilized the WO_3 crystal lattice. The symmetry phase transition to the highly ordered WO_6 octahedra has been confirmed also by the IR spectroscopy. The results of the diffuse reflectance spectroscopy show that all the synthesized W/Ti oxide materials possess a visible-light band gap (2.72–2.82 eV). Five pharmaceutical compounds have been selected to evaluate the possible photocatalytic activity of the W/Ti oxide samples under solar illumination. The first photocatalytic experiments have been performed with the W/Ti 10:1 oxide powder and the results confirmed that degradation of hydrophilic pharmaceutical compounds takes place. More detailed study is underway and will be presented. We aim to evaluate to what extent the incorporation of Ti into the WO_3 – which strongly influences the structural and optoelectronic properties of the material – influences the photocatalytic activity, i.e. photodegradation of the pharmaceuticals, compared to the pristine WO_3.

Keywords: photocatalysis, tungsten(VI) oxide, solar light, contaminants of emerging concern

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Comparison of active ingredients' concentrations in the wastewater of two hospitals

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The growing global population, advances in research, increased investment in the pharmaceutical industry and the widespread availability of medicines are driving a significant rise in the consumption of medicines. Active pharmaceutical ingredients (APIs) are inherently biologically active and are designed to resist biodegradation, as metabolic stability typically enhances their desired pharmacological activity. This contributes to their environmental persistence [1]. Analysing pharmaceutical contaminants in water is challenging because of the complex matrix and low concentrations of target substances. Hospital wastewater contains hazardous chemicals, solvents, active substances, metabolites, disinfectants, and heavy metals, which can persist in the environment for a long time and pose serious threats to nature and have high mobility in the liquid phase.

The aim of the study was to analyse and compare the presence of selected active ingredients in wastewater (WW) from a rehabilitation hospital in Austria and a general hospital in Slovenia. The results of the WW samples show that several APIs were detected in WW from both hospitals. The highest concentrations were recorded in the WW for caffeine as well as for cardiovascular and nervous drugs in all tested wastewaters. The APIs, such as ibuprofen, paracetamol, theophylline and caffeine were determined in all eight WW samples taken from both hospitals. The results agree with other studies where among the most frequently detected pharmaceuticals in aquatic environment non-steroidal anti-inflammatory drugs (NSAIDs) such as ibuprofen, diclofenac, and naproxen due to their extensive use in the treatment of pain, inflammation, and fever [2]. Investigated wastewater effluents are not purified on treatment plants to completely remove complex compounds, before release into the environment.

Keywords: Active pharmaceutical ingredients (APIs), hospital wastewater, enviromental impact, analytical methods, NSAID (non-steroidal anti-inflammatory drugs)

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Cytocompatibility Assessment of 3D-Printed Resins for Bone-on-a-Chip Applications Using Human Osteoblasts

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Understanding bone physiology and pathology is of major scientific and clinical importance. As the body's primary load-bearing tissue, bones support movement, maintain mineral balance, and provide a niche for bone marrow, which produces mesenchymal stem cells and hematopoietic progenitors. Traditional studies on bone development and related diseases relied on 2D cultures, 3D in vitro models, or animal experiments, but all fall short in fully replicating human bone physiology. The next step in evolution is organ-on-a-chip (OoC) models, which are driven by advances in microfluidics and promise to fully address past limitations. These miniaturized systems offer precise control over microenvironmental factors (e.g., oxygen levels, cytokine gradients, mechanical stiffness, shear stress, and loading), creating more physiologically relevant conditions than conventional cultures. Among examples are also bone-on-a-chip (BoC) platforms for more accurate bone biology studies [1]. A critical aspect of BoC design is selecting materials that effectively mimic the bone microenvironment. Polydimethylsiloxane (PDMS) is widely used due to its biocompatibility, transparency, elasticity, gas permeability, and affordability. However, PDMS can absorb small hydrophobic molecules, potentially interfering with media components and drug testing accuracy [2]. With rapid advances in 3D printing, new materials that better simulate bone properties have become available. As with all biomedical materials, biocompatibility is essential to minimize adverse effects on cells, as well as to allow for relevant testing outcomes. Due to the continuous emergence of novel commercial resin-based materials, data on their cytotoxicity remains limited. As such, many resins lack thorough biosafety testing, which hinders their use [3].

In this study, we evaluated the biocompatibility of commonly used photopolymer resins in general and dental 3D printing (S200 Standard Resin, PH100 eResin-PLA Pro, and DM100 Dental Restoration Model Resin) using human fetal osteoblast (hFOB) cells. Cytotoxicity was assessed via direct and extract-based MTT assays following ISO 10993-5:2009 standards, along with a live/dead viability assay. Cell morphology was examined using phalloidin staining to visualize actin filaments. The goal was to assess the cytocompatibility of these resins and explore the relationship between leachable components and osteoblast damage. To our knowledge, this is the first comprehensive study evaluating the biological risks of resins in 3D-printed BoC devices.

Acknowledgements

The authors acknowledge the financial support from the Slovenian Research Agency for Research Core Funding No. P3-0036, and for projects Nos. L7-4494, J1-60015 and J3-60058.

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Supercritical CO_2 Extraction and Characterization of Volatile Compounds and Fatty Acids from *Epilobium parviflorum*

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Epilobium parviflorum is a perennial plant of the willowherb family (*Onagraceae*). It is native to Europe and parts of Asia and is often found in damp, grassy places such as riverbanks and meadows. *Epilobium parviflorum* is traditionally used as a medicinal plant and has attracted attention for its potential anti-inflammatory, antioxidant, antimicrobial and antiproliferative properties. It contains several bioactive constituents, including flavonoids, tannins, phenols, phytosterols, terpenoids and fatty acids, which may have a positive effect on human health [1]. In recent years, the extraction of natural substances with supercritical fluids has become increasingly popular. CO_2 is often used to extract bioactive components from biomass without hazardous chemical processes, as it is non-toxic, non-flammable, thermodynamically stable and has a low critical point, which is also favourable for the isolation of thermolabile components. By avoiding the use of organic solvents, $SCCO_2$ offers a safer and more environmentally friendly alternative for the extraction of essential oils, lipids and other bioactive substances [2].

Supercritical CO_2 was used for the extraction of volatiles and fatty acids from *Epilobium parviflorum*. Previously ground dry leaves and stems of the plant were treated with $SCCO_2$ at 300 bar, 40 °C and a CO_2 flow rate of 1.3 kg/h. The yield of volatiles, lipids and other bioactive components obtained by $SCCO_2$ extraction was 0.25 %. The $SCCO_2$ extract was further characterised by headspace solid-phase microextraction coupled with GC-MS for volatiles and GC-FID for fatty acids. The fatty acid profile of the $SCCO_2$ extract showed that the most abundant fatty acid was linoleic acid (42.92 %), followed by α-linolenic acid (17.63%), palmitic acid (17.19 %) and oleic acid (12.96 %). Analysis of the volatile components of the extract revealed the presence of groups of phenol derivatives, terpenoids and terpenes, aldehydes, ketones, alcohols and carboxylic acids. The main constituents were a group of phenol derivatives with the main components anethole (27%) and estragole (3%) and terpenoids with carvone (18%) and pulegone (2%). Based on the biocomponent profiles, it can be concluded that the $SCCO_2$ extract of *Epilobium parviflorum* is potentially beneficial to health.

Keywords: *Epilobium parviflorum*, supercritical CO_2, extraction, volatiles, fatty acids

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Preparation of pectin gels for the stabilisation of natural colorants from aronia fruit residue

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Pectins represent a diverse group of anionic, water-soluble heteropolysaccharides whose characteristic structural backbone consists of α-1,4-linked D-galacturonic acids (GalA) [1]. As macromolecular polysaccharides, they are widely distributed in the middle lamella and primary cell walls of dicotyledonous and non-grassy monocotyledonous plants and act as hydration agents [2]. Commercially, pectin is mainly extracted from citrus peel and apple pomace and is used in the food and pharmaceutical industries as a gelling, stabilising, thickening, emulsifying and colour protecting agent as well as in drug delivery applications, where the gelling properties of pectin are very important [1]. The gelation of pectin is significantly influenced by the molecular structure (degree of methylation and acetylation, molecular weight, heterogeneity of the polymer chains), the pectin concentration, the presence of cross-linking agents, the temperature, the pH value and the ionic strength [1, 2, 3]. *Aronia melanocarpa* berries (aronia berries) are a very rich source of natural antioxidants, which have a major positive impact on human health [4]. Aronia is often processed into fruit juice and the residues of the berries are used for various purposes. Aronia berries contain a large amount of natural colorants, anthocyanins, which can be isolated from the fruit processing residues [5].

In the present contribution, the preparation of pectin gels from high methoxy pectin was carried out to stabilise the natural colourants from the aronia berry residues. In the first part of the study, the influence of the gelling parameters, the type of crosslinker added, the concentration of the crosslinker and the pH of the solution were tested to produce a stable pectin-based gel. The inverted tube method was used as a rapid scanning method of the gelation profiles. The chemical structure and microstructure of the pectin gels were characterised by FTIR and SEM. In the second part of the study, natural colourants were isolated from aronia berries residue and incorporated into pectin gels. The influence of the natural colourants on pectin gel formation was investigated and the stability of the pectin-anthocyanin gels was tested using the inverted tube method, FTIR and visual and spectrophotometric observation.

Keywords: pectin gel, stabilization, natural colorants, *Aronia melanocarpa*, fruit residue.

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Molecular Insights into Lipase Thermostabilization by Deep Eutectic Solvents

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Deep eutectic solvents (DES) are a new class of green solvents that have enormous potential in several fields like organic and material chemistry, electrochemistry and catalysis as well as extraction processes and dissolution [1]. They are mixtures of two or more compounds – a hydrogen bond donor (HBD) and acceptor (HBA) – that upon interaction, form a liquid whose eutectic point is below the temperature of an ideal liquid mixture [2]. The properties of these solvents are highly tuneable and their low toxicity, high solubilizing capacity and stabilizing nature, makes them suitable solvents for enzymatic reactions [3]. The protein-stabilizing effects of DES are reflected in their significant thermostabilizing capacity that enables enzymatic reactions at elevated temperatures and subsequent higher product yields [4].

In our study, we aimed to determine the role of individual DES components on the thermal stability of lipase. Lipase B from *Candida antarctica* was incubated in DES composed of choline chloride (ChCl) or betaine (Bet) as HBAs and urea (U), glycerol (G), sorbitol (Sorb) or xylitol (Xyl) as HBDs at 80°C. Tris/HCl buffer served as a reference solvent. Water was added to the DES in varied amounts, from 5 wt% to 75 wt%. The results showed that the addition of 10 wt% of water was the most beneficial in regard to thermal stabilization, with relative activity (RA) of 8 to 10-times higher compared to buffer. Higher water amounts resulted in the weakening of the DES H-bond network and, subsequently, lower thermostabilizing capacity. At 75 wt% water amount, the effects of individual components became more evident. Thus, the thermostabilizing effects of ChCl, Bet, G and U with 25 and 75 wt% of water were tested and compared to respective DES. The results showed a complex relationship between the individual components. ChCl had a strong thermostabilizing effect (RA = 11) on lipase whereas, U had an inhibitory effect (RA = 1), but when combined in a DES, they showed potential synergistic effect (RA = 12). On the other hand, combining ChCl with G in a DES, resulted in lower RA (RA = 9) compared to only ChCl, although G by itself, had some thermostabilizing properties (RA = 4). In the case of Bet (RA = 5), the combination with G in a DES, resulted in higher thermal stabilization (RA = 7). Again, all solutions (individual compounds or DES mixtures) performed better with a lower amount of water (25 wt%). To investigate the stabilizing effects of individual components on the enzyme, molecular docking calculations were performed. We used ChCl, Bet, U, G, Sorb, and Xyl together with Tris and its protonated form (Tris+), and performed calculations on the surface of the whole enzyme (*Candida antarctica* lipase B, PDB ID 1TCA [5]) as well as the active site of the enzyme. The simulations showed that ChCl forms H-bonds with the protein near its active site, which is likely the reason for ChCl's high thermostabilizing capacity. On the other hand, binding of Bet occurred far away from the active site, which offered no direct effect on the structure of the enzyme's active site. The preferred binding site of all HBDs was located outside the enzyme's substrate binding site and binding was relatively weak resulting in lower thermostabilizing effect. All of the compounds preferentially bound outside of the active site, which suggested that it is not likely that they affect enzyme activity through competitive binding. These results offer an insight into the DES's stabilization capabilities on the atomistic level, however, in order to gain a detailed understanding on stabilization mechanisms, more extensive simulations of lipase solvated in various DES compositions and concentrations are required.

Keywords: Lipase; Deep eutectic solvents; thermostabilization; molecular docking

Acknowledgments
This research was funded by the Slovenian Research and Innovation Agency within the projects P2-0152 and P2-0421.

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Vpliv pH na izomerizacijo kohumulona

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Hmelj je industrijsko pomembna rastlina, ki se uporablja pri varjenju piva. Najpomembnejše polifenolne spojine, ki jih najdemo v hmelju, so: ksantohumol, α-kisline in β-kisline. Pri varjenju piva je vsebnost ksantohumulo in β-kislin v hmelju manj pomembna, saj ksantohumul ne prispeva bistveno k okusu piva, medtem ko β-kisline med varjenjem piva razpadejo. Vsebnost α-kislin v hmelju pa je ključnega pomena za končni okus piva, saj α-kislin med varjenjem piva izomerizirajo v cis- in trans-izo-α-kisline, ki povzročijo grenak okus piva. Poleg tega so te spojine pomembne tudi za stabilnost piva, saj delujejo protimikrobno.

S tehnološkega vidika je izjemno pomembno dejstvo, da se le del α-kislin pretvori v izo-α-kisline. Izkoristek pretvorbe pa je močno odvisen od pogojev varjenja piva. Poleg tega pa razmere v raztopini vplivajo tudi na to, kolikšen delež α-kisline se bo pretvoril v cis-izo-α-kislin in kolikšen delež v trans-izo-α-kisline. Zato ni presenetljivo, da obstajajo številne študije, ki se ukvarjajo z izkoristkom in kinetiko izomerizacije. [2] Večina teh študij je zastavljena tako, da kar se da dobro posnemajo pogoje, pri katerem poteka varjenje piva, medtem ko so sistematične fizikalno-kemijske študije redke [3].

Študijo smo začeli z izolacijo α-kisline kohumulona iz hmelja, z uporabo reverznofazne tekočinske kromatografije visoke ločljivosti. Nato smo z uporabo spektroskopije UV/Vis in izračunov DFT določili, na katerih mestih pride do prve in druge deprotonacije. [1] Nato smo z uporabo spektroskopije UV/Vis in kromatografije HPLC preverili, kako pH vpliva na hitrost izomerizacije kohumulona v izo-kohumulon. Z uporabo kromatografije HPLC smo preverili tudi, kolikšen delež kohumulona se pretvori v cis- in trans-izomero. In seveda, ali poteka še kakšna konkurenčna reakcija. Dobljene rezultate smo nato korelirali z deležem posamezne zvrsti v raztopini, s čimer smo dobili boljši vpogled v mehanizem izomerizacije hmelja.

Ključne besede: hmelj, kohumulon, kinetika izomerizacije,

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Ammonia Absorption in Silica: Development of a New ReaxFF Potential

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Ammonia, a small molecule of great potential. Despite its importance for industry and being a key molecule in the "Green revolution", the ammonia synthesis has remained largely unchanged for more than a century since Haber and Bosch developed the ammonia synthesis for industrial purposes [1.2]. Numerous studies, both experimental and theoretical [3,4], have been orientated towards discovery of novel catalysts, yet the process remains largely unchanged. In an alternative approach, the yield of the ammonia could be increased, by replacing the condenser with a bed of solid absorbent in which ammonia is absorbed, thus removing in it from the reaction mixture and moving "the equilibrium" towards the products. The absorbent captures produced ammonia in a solid crystal and is superior to an adsorbent in two ways, (i) ammonia is captured at higher temperatures and (ii) it is more selective [4]. Additionally, the amount of ammonia absorbed is much higher than the one expected for adsorption. Namely, in the case of adsorption, ammonia is adhered only to the crystal structure, while when being absorbed it penetrates significantly in the solid.

Understanding the mechanism of work of silica-based ammonia sorbents could pave the road toward improved and energetically less demanding ammonia synthesis. Here, we used multiscale approach to (i) test different density functional theory (DFT) methods and basis sets to determine most favourable ammonia absorption sites on the non-defective and defective silica surface models and (ii) use obtained data to develop a novel reactive force field (ReaxFF) potential, called ReaxFF^{SiONH3}, describing ammonia-silica gas-surface interactions. Empirical potential-based molecular dynamics simulations have previously been developed and used to study gas-surface interactions between silica and oxygen and ruthenium and ammonia, however, the ReaxFFs, which are classified as empirical based force fields, are highly system specific and can be used only to study systems which are similar to the ones that ReaxFF was parametrized for. The obtained interaction energies from ReaxFF^{SiONH3} are in good agreement with the density functional energies and can now be used in reactive large-scale molecular dynamics simulations aimed at understanding the ammonia absorption mechanism in real porous silica surfaces.

Keywords: DFT, classical molecular dynamics, ammonia absorption, silica, reactive force field

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A Theoretical Study of Mass Transport Mechanisms in Porous Membrane Distillation Modules

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Membrane distillation is a separation technology that uses low grade heat such as industrial waste heat or solar energy to power the distillation process. High salinity solutions can be distilled using a hydrophobic porous membrane that rejects non-volatile species [1]. The difference in pressure is the driving force of vapor transport between the hot feed solution and cold permeate membrane boundary. Theoretical modeling of membrane characteristics is used to calculate total membrane mass transport. Current configurations of membrane distillation systems and low membrane mass flux call for process optimization. The flux can be determined theoretically from membrane properties. Different models can be applied to the membrane characteristics to evaluate the theoretical models [2], [3].

First, a geometric model of a direct contact membrane distillation (DCMD) module was developed to represent the geometrical configuration of the system. This model served as the basis for a CFD (Computational Fluid Dynamics) simulation, which was carried out to analyze the fluid flow and heat transfer within the membrane module. Temperature profiles were extracted from the simulation results, providing boundary conditions for the subsequent modelling of mass transfer. Based on the temperature data, a comprehensive theoretical model was created to estimate the total mass flow through the membrane. Membrane properties such as tortuosity, effective diffusivity, diffusion and thermal resistance were integrated into this model to account for the complex transport phenomena within the porous structure. The mass transport mechanism was described using the Dusty Gas Model (DGM) in and the Maxwell–Stefan diffusion equations.

The theoretical flux predictions of the model were then compared with experimental data from the literature to validate the approach. This comparison helped to evaluate the accuracy and reliability of the proposed.

Keywords: diffusion modelling, membrane distillation, computational fluid dynamics

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Modeling of high-temperature radical copolymerization of dibutyl itaconate with styrene and terpolymerization of dibutyl itaconate, n-butyl acrylate and styrene

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Acrylic resins are essential for protective coatings in various industries, but their conventional raw materials are mostly fossil-based and expensive to replace with bio-based alternatives. Itaconate diesters, derived from renewable sources, offer a promising, fully sustainable option for improving the environmental profile of acrylic polymers without compromising their key properties. The copolymerization kinetics of itaconates are still poorly understood, although it has long been known that their homopolymerization results in low monomer conversion rates and reduced polymer molecular masses. The key reasons is that depropagation significantly influences the radical polymerization of itaconates even at temperatures below 100 °C [1,2].

Previous studies have shown that the copolymerization of dibutyl itaconate (DBI) with butyl acrylate (BA) results in high conversions and relatively long polymer chains, while copolymerization with styrene (St) leads to slightly lower conversions but on average longer polymer chains [1,2,3]. It has been found that during the copolymerization of itaconates with methyl methacrylate (MMA), the presence of the MMA further accelerates depropagation [4]. Therefore, our experiments were performed to research the terpolymerization of DBI, BA, and St at different feed compositions of the introduced monomers, keeping the DBI mass fraction relative to the total monomer content constant at 50 %. Starved-feed solution terpolymerization processes were carried out in semibatch reactors, which enable controlled heat release, provide control over the polymer composition and allow system modeling [5]. We also carried out modeling of the copolymerization of DBI with St, investigating how well the experimental results can be approximated using the terminal model.

Keywords: Dibutyl itaconate, Modeling, Terpolymerization

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Comparison of HDPE polymer and HDPE plastic bottle caps

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Plastic has become one of the most important materials in recent decades. However, most plastics are of synthetic origin and diminish into smaller units (microplastics) over time, which has a negative impact on the environment and subsequently on human health. The most common methods of plastic recycling today are mechanical and chemical recycling. Recently, however, more and more emphasis has been placed on the upcycling of plastic waste into higher value products [1, 2]. HDPE is one of the most commonly used plastics as packaging material due to its good properties such as hardness, low cost, flexibility and recyclability. Plastic bottle caps rank among the top five most frequently found litter items on beaches around the world. In 2016, a large study was conducted in the Netherlands on the pollution of beaches by plastic bottle caps, in which more than 10,000 bottle caps were collected, categorized and analyzed [3]. In addition, it has been already proved in literature that also colorants and additives have a significant impact on thermal and catalytic pyrolysis and environmental degradation [4].

In this study, we focused on the characterisation of virgin HDPE polymer in granular form (without additives) and two different green and pink HDPE bottle caps obtained from Radenska and Lissa bottled water using thermal and rheological characterization techniques. The dynamic scanning calorimetry (DSC) analysis showed that the start of melting temperature (T_{onset}) obtained from 2nd heating was the highest for the virgin HDPE and the lowest for the green bottle caps. Thermogravimetric analysis (TGA) showed that the HDPE sample exhibited a mass loss of approximately 99.7% at 600 °C, whereas the mass loss for both analyzed bottle caps was slightly lower, by less than 1%. Furthermore, flow behaviour of virgin HDPE polymer melt at 140, 150 and 160 °C differed from that of the HDPE bottle caps. The viscosity of polymer melts decreased with increasing measurement temperature. The results show that the differences in thermal as well as rheological properties between virgin HDPE and the two HDPE bottle caps can be attributed to the use of different pigments and/or different additives in the processing/production of the bottle caps.

Keywords: HDPE, bottle caps, thermogravimetric analysis (TGA), differential dynamic calorimetry (DSC), viscoelastic properties

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Polypyrrole and Graphene Additives for Conductive Natural Rubber Composites: Role of Electric Field Orientation

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Conductive elastomers composed of natural rubber latex (NRL) and conductive fillers were investigated with the aim of enhancing their electrical conductivity. The conductive fillers used in this study included graphene nanoplatelets (GNP), a commercially available multisheet graphene conductive additive (GCA), and polypyrrole (PPy), which was synthesized according to a method described in the literature [1]. As the base material, we used commercially available prevulcanized natural rubber latex (Gumiform, 61% dry matter), supplied by Samson Kamnik.

Conductive fillers were added to the liquid latex to obtain NR samples containing various weight percentages of filler, calculated relative to the dry matter content of the latex. The fillers (1-10 wt%) were dispersed into the latex matrix by magnetic stirring. The resulting dispersions were cast into molds and left to dry in ambient conditions to produce solid samples named as NR+X%Filler. Additionally, sample NR+10%PPy was subjected to different electric voltages (from 1 V to 100 V) before drying, to examine its effect on possible orientation or distribution of the conductive filler within the latex and thus its influence on the conductivity of the dried sample.

Pure NR elastomers showed very high resistivity. The addition of small amounts of GNP (up to10 wt%) did not significantly affect the resistivity, indicating that a percolation threshold was not reached [2]. However, a more noticeable reduction in resistivity was achieved using 10 % of the GCA and synthesized PPy. Furthermore, exposing the NR+10%PPy liquid sample to an electric field ranging from 1 V to 100 V before drying resulted in a substantial decrease in resistivity. The results showed that mere addition of nanoscale conductive fillers, such as graphene nanoplatelets, does not necessary lead to significantly enhanced conductivity of NR-based composites. In contrast, exposure of PPy-filled latex to an electric field before drying promoted the alignment of conductive particles along the direction of the electric current, enhancing the formation of conductive pathways and thus lowering the overall resistivity of the dried elastomer.

Keywords: natural rubber latex, graphene nanoplatelets, polypyrrole, conductivity.

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Antioxidant and antimicrobial properties of aronia pomace extract

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The growing demand for sustainable and health-conscious materials has intensified research into agro-industrial by-products as low-cost, renewable sources of bioactive compounds. Recent studies have demonstrated that fruit extracts of *Aronia melanocarpa* significantly enhance dyeing performance and impart functional properties to cotton fabrics [1]. Moreover, residues from *A. melanocarpa* processing, particularly pomace, represent a valuable source of bioactive compounds, with higher polyphenol bioaccessibility compared to leaves [2]. In this context, aronia pomace, a solid by-product generated during juice production, was evaluated as a multifunctional colourant for textile printing applications.

To extract the active compounds, the pomace was subjected to ultrasound-assisted maceration, and the resulting extract was characterised using gas chromatography–mass spectrometry (GC/MS). Antioxidant and antimicrobial properties were evaluated, revealing a rich polyphenolic profile, similar to that of grape pomace extract [3]. Antioxidant assays confirmed notable radical-scavenging activity, while antimicrobial screening via the agar dilution method showed inhibitory effects against *Staphylococcus aureus*, *Escherichia coli* and *Candida albicans*, indicating good antimicrobial potential.

The extract was mixed into a sodium-alginate screenprinting paste and printed onto a plain weave cotton fabric. After printing, colour was measured using a Konica Minolta 2600d spectrophotometer. The mean CIELab coordinates of printed samples were showing a red shade with a slight blue undertone. Spectral reflectance curves showed pronounced absorption from 360 to 560 nm, with a maximum at 540 nm (K/S = 2.5).

These findings suggest that aronia pomace extract can be an eco-friendly solution for developing antibacterial and antioxidant-treated textiles, with potential applications in healthcare and protective clothing.

Keywords: aronia pomace; antibacterial activity; antioxidant properties; anthocyanins; screenprinting.

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Antimicrobial and Antioxidant Activity of *Helichrysum Italicum* for Potential Applications in the Cosmetic Industry

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Due to the great awareness of the need for skin care, the number of consumers in the cosmetics industry is growing. At the same time, the need for products with proven effective natural active ingredients and the elimination of unnatural alloys (e.g., parabens, silicones, artificial colors, and synthetic fragrances) is growing. The native Mediterranean plant of immortelle (*Helichrysum. italicum* (Roth) Don) is an outcrossing plant, which grows widely in natural, different and fragmented habitats in dry and sandy-rocky areas of Mediterranean regions. Immortelle represents a rich reservoir of numeral phytochemicals possessing several biological properties, including antimicrobial, antiinflammatory, antioxidant, antiviral, anticarcinogenic, antilarvicidal, and repellent activities [1–2]. It can be used to obtain medicinal extracts/hydrolates/essential oils with antimicrobial and antioxidant effects. Nowadays, the essential oil of immortelle is very appreciated for the perfume and cosmetic industry due to anti-ageing properties. The high value of biologically active substances from *H. italicum* is attributed to various extracts prepared from different parts of the plant, which chemically differ depending on the extract preparation, the origin of plant material (leaves, stems, flowers), the developmental stage of the plant, and plant taxonomy. Besides the usage of standard solvents, using supercritical carbon dioxide (SC CO_2) gives a “green” solution to obtain valuable biocomponents. Extraction from biological material using supercritical fluids (SCFs) is nowadays an industrially recognized method and represents an alternative process to conventional extractions, suitable for isolation of natural thermolabile substances.

Hydrolates and essential oil from *H. italicum* hybrids, as well as extract from *H. italicum* obtained by supercritical SC CO_2 extraction (SFE) were tested on antioxidant and antimicrobial activity. The highest antioxidant activity detected by using DPPH method was in SFE extract, followed by hydrolate and essential oil from *H. italicum.* The SFE extract was also the most promising antimicrobial agent, as it preliminarily inhibited all selected microorganisms and generally showed the lowest MIC values for all tested microorganisms.

Keywords: *Helichrysum italicum*, extract, essential oil, antimicrobial, antioxidative

Acknowledgement: This research was supported by the Slovenian Research Agency (ARRS) within the frame of program P2-0046 (Separation Processes and Production Design), and project No. L2-4430 (Production, Isolation and Formulation of Health Beneficial Substances from *Helichrysum italicum* for Applications in Cosmetic Industry).

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Carbon Reinforced Polycarbonate Recycling with Subcritical Water

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The use of carbon fibre reinforced plastics (CFRP) has increased exponentially over the last decade. Due to their mechanical properties, they are used in a wide range of industries, particularly in the aerospace and automotive industries. The exponential increase in the use of CFRP poses a major problem for the environment as much of the waste ends up in landfill. The only way to avoid further landfill and reduce the impact on nature caused by the increasing use of CFRP is recycling [1].

Hydrothermal processes for the degradation of carbon fibre reinforced polycarbonate use water at high temperatures and pressures, but below critical water conditions. Under such conditions, water has a low viscosity, a high diffusivity and a high ionization constant, which significantly increases the ability to degrade organic components. The use of water as a solvent has other advantages, such as rapid hydrolysis without the need for catalysts and high monomer yields. In addition, water is a cheap reagent and, above all, its use is environmentally friendly [2].

In this study, the decomposition of carbon fibre reinforced polycarbonate (with 30% carbon fibres) in subcritical water was investigated to determine optimal reaction conditions, in particular temperature and time, for the recovery of valuable products. The experiments were carried out in a batch reactor at temperatures between 250 °C and 350 °C and reaction times between 5 and 120 minutes. Subcritical water effectively decomposed polycarbonate into valuable compounds, including bisphenol A (BPA), various alkylphenols and phenol. Analysing the influence of temperature and time showed that the highest yield of these products (63.8 %) was achieved at 300 °C and 30 minutes. These results emphasise the crucial role of the process parameters in determining the reaction pathway, the product types and their respective yields.

Acknowledgement: The authors would like to acknowledge the Slovenian Research Agency Research Core Funding no. P2-0421 (Sustainable Technologies and Circular Economy) for financing this research and young researcher fellowship awarded to M.I.

Key words: carbon reinforced plastic, subcritical water, chemical recycling, bisphenol A, hydrothermal process

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Recycling copper from fish farming nets

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The company AquafilSLO, part of Aquafil Group, has been operating its chemical recycling of PA 6 from waste based on depolymerisation for several years. One of the products that can be recycled through this process are fish farming nets. However, these nets are treated with a biocidal coating containing a copper-based active substance, which prevents biofouling (the adhesion of microorganisms) and extends the nets' operational life.

For this reason, a pre-treatment step involving the washing of the used nets is essential. The washed PA 6 from the nets proceeds to the depolymerization reactors for chemical recycling, while the remainder is a sludge that contains approximately 25% copper in its dry matter. As copper in specific forms can be a valuable and useful raw material, we partnered with Cinkarna Celje to explore the possibilities of recovering copper from the sludge.

Cinkarna Celje, specialized in production of copper-based plant protection products, has been researching several treatment methods for recovering of copper from the sludge in the forms apt for production of the new antifouling coating for the nets.

The newest treatment method being developed by Cinkarna Celje is anticipated to be the most effective, as it aims to reduce the number of steps and consumption of auxiliary materials. The sludge produced from washing the fishing nets is very sticky, which makes any handling of it challenging.

The core of the proposed new idea is that the sludge remains inside a big bag throughout the entire treatment. The big bag is placed into a special leaching apparatus and is rinsed with hydrochloric acid. In this process, copper is leached out in the form of copper chloride. Once all the copper has been leached, the remaining filter cake is washed with water and dewatered (pressed) to remove any final traces of copper. The copper- and chlorine-free filter cake is then sent for incineration along with the big bag.

The advantage of this process over dissolving thermally treated sludge is that it avoids the release of gaseous HCl, which is highly aggressive at high temperatures. Furthermore, in conventional thermal treatment, HCl is first removed and must then be re-added as hydrochloric acid to dissolve the resulting copper oxide. The innovative sludge leaching process is therefore more favourable in terms of material consumption.

Based on the recovered, regenerated copper chloride solution, the active substance copper oxychloride is synthesized, which can be reused for treating fishing nets. Through this additional pretreatment and recovery process and collaboration, a closed loop is achieved not only for the PA6 but also for the copper by-product improving the method of recycling of waste fish farming nets.

Keywords: PA6, copper, fishing nets, recycling, coating, biocide

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Circular Economy Concepts at Cinkarna Celje

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Cinkarna Celje, a Slovene producer of titanium dioxide pigment using the Sulphate route, is implementing various circular-economy strategies to lower resource consumption and waste generation, while also developing a broader product portfolio. Cinkarna Celje is developing and establishing four different pillars of circular economy.

The first pillar is integrated water management: investments in infrastructure that enable most process water to be treated or simply returned to the system, significantly reducing extraction from the local river all while maintaining wastewater monitoring to protect local ecosystems [1]. These measures are expected to decrease reliance on natural water sources and improve resilience to climate variability [1].

The second pillar is focused on valorising 23 % waste sulphuric acid that is the effluent coming from TiO_2 production. The established process of acid neutralization is used to produce white gypsum, which is marketable (CE-gips) and red gypsum (RC-gips), the latter being landfilled. Valorisation of the 23 % waste acid stream using selective precipitation approaches enables an increase in the specific amount of produced white gypsum, while simultaneously decreasing the landfilled red gypsum. Furthermore, the valorisation approach enables us the extraction of Ti (IV) values, which complement our production capacity, recovery of iron as ferric oxalate, and extraction of vanadium and scandium values [2].

A third circular-economy initiative concerns the mineral residue left after acid leaching of ilmenite and titanium slag. A new approach of residue processing has been developed that enables the extraction between 65 and 75 % of titanium dioxide, while reducing waste by up to 65 % [3]. Implementing such technology further decreases waste and enables the recovery of Ti (IV) that are now partially lost with landfilling the mineral residue.

These fourth pillar is the use of red gypsum as a secondary raw material for sustainable construction applications. Current results demonstrate red gypsum's potential as a low-carbon additive in construction materials and support its integration into circular economy strategies.

These initiatives show how an established chemical company can reduce environmental impacts and create value from residual streams. Integrated water recycling, waste-acid valorisation, ore-residue processing and red gypsum valorisation are central to Cinkarna Celje's strategy for a more circular and resilient titanium dioxide production.

Keywords: circular economy; integrated water management; waste acid valorisation; gypsum recovery; ore-residue processing

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Sustainable Construction Composites Based on Red Gypsum from Cinkarna Celje

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Red gypsum (RG) is an industrial by-product of titanium dioxide production via the sulphate route and is mostly landfilled, despite its mineralogical composition that includes calcium sulphate, iron oxides, and residual titanium dioxide [1,2]. In light of circular economy strategies and the growing need for low-carbon construction materials, RG has emerged as a promising candidate for environmentally assessed waste (EAW) valorization

In this study, red gypsum (RG), an industrial by-product from titanium dioxide production at Cinkarna Celje d.d., was evaluated as a secondary raw material for sustainable construction applications. The material was chemically and physically characterized and incorporated into both cement-based and alkali-activated (geopolymer) systems [3].

In cementitious composites, Portland cement CEM I 52.5 R was used as the main binder. Red gypsum (RG) was dried, milled, and sieved to <90 µm, then added in 5–20 wt% proportions. Lower additions (5–10%) slightly delayed setting but maintained compressive strength above 60 MPa after 28 days, confirming RG's potential as a functional additive without compromising structural integrity. FTIR-ATR and Le Chatelier tests indicated good chemical and dimensional compatibility. As a sand substitute, RG significantly reduced strength and proved less suitable. In metakaolin-based geopolymer composites, RG retained sufficient compressive strength for non-structural applications.

The results demonstrate RG's potential as a low-carbon additive in construction materials and support its integration into circular economy strategies.

Keywords: red gypsum, secondary raw material, cementitious composites, geopolymer materials

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Termo-kemična obdelava industrijskih odpadkov

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Biomasa je pomemben obnovljiv vir energije, ki je globalno dostopen in lahko pripomore k zmanjševanju neto emisij CO_2. Posebej obetavna je energetska izraba industrijskih odpadkov, saj omogoča hkratno zmanjšanje količine odpadkov in pridobivanje sekundarnih surovin. Vendar pa surova biomasa pogosto ni neposredno primerna za uporabo kot gorivo, zaradi nizke energijske gostote, visoke vsebnosti vlage ter nehomogene sestave. Za izboljšanje lastnosti takšnih materialov je potrebna ustrezna predobdelava [1]. Med postopki, ki omogočajo takšno predobdelavo, izstopata torefikacija in hidrotermalna karbonizacija (HTC). Oba procesa vodita v proizvodnjo trdnega produkta z izboljšanimi gorivnimi lastnostmi ter večjo stabilnostjo, kar pripomore k večji učinkovitosti pri energetski izrabi. Zaradi svoje preprostosti in učinkovitosti predstavljata obetavno rešitev za valorizacijo nizkokakovostnih biomaterialov [2,3].

V raziskavi smo preučevali možnosti energetske izrabe ostankov iz različnih industrijskih procesov. Kot izhodiščne materiale smo uporabili rožmarinovo pogačo, rožmarinove tropine, jabolčne tropine in grozdne pečke. Namen raziskave je bil ovrednotiti vpliv dveh termo-kemičnih postopkov, torefikacije in hidrotermalne karbonizacije, na kakovost nastalih trdnih produktov z vidika njihove uporabnosti kot alternativna goriva. S torefikacijo smo pridobili bio-oglje, s hidrotermalno karbonizacijo pa hidro-oglje in procesne tekočine. Torefikacijo smo izvedli pri 250°C v inertni atmosferi dušika. Hidrotermalno karbonizacijo smo izvedli pri 260°C, pričemer smo kot tekoči medij uporabili odpadno vodo iz procesa proizvodnje rožmarinovih ekstraktov z namenom, da bi znižali porabo sveže vode v procesu. Karakterizacijo surovin in pridobljenih trdnih produktov smo izvedli s proksimativno analizo, FTIR spektroskopijo ter določitvijo zgornje kurilne vrednosti. Poleg tega smo za podrobnejši vpogled v termično stabilnost vzorcev uporabili termogravimetrično analizo (TGA) v dušikovi atmosferi, z vzporedno identifikacijo nastalih plinov s pomočjo tehnike TGA-FTIR. Analizirali smo tudi procesne tekočine procesa HTC, s čimer smo preučili vpliv hidrotermalne obdelave posamezne vrste biomase na sestavo procesne tekočine.

Ključne besede: termična obdelava, industrijski odpadki, torefikacija, hidrotermalna karbonizacija, termogravimetrična analiza

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Ecotoxicological aspect of PET plastic waste use in concrete as partial aggregate replacement

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Over the past decade, various strategies for reducing plastic waste have been proposed. One particularly promising approach involves incorporating PET plastic waste into concrete as a partial replacement for natural aggregate. While the ever-increasing concrete production depends on natural resources, PET plastic waste as an aggregate could contribute to both the reduction of natural resources consumption and PET plastic waste [1]. Past research has shown that replacing up to 5% of natural aggregate with PET particles in concrete either has no significant impact or may even enhance the mechanical properties compared to conventional concrete [2]. However, throughout its service life, concrete is exposed to diverse environmental conditions, and the inclusion of PET raises concerns about the potential leaching of toxic substances. Therefore, the ecotoxicological assessment of such material is as important as the determination of mechanical properties to predict the impact of leachates of such material on the ecosystem, especially if such material would one day become waste [2,3].

This study aimed to assess both the mechanical and ecotoxicological properties of concrete in which PET plastic waste replaced 5% of natural aggregate. Preliminary results PET plastic waste-containing concrete and conventional concrete had comparable mechanical properties. Ecotoxicity test results using mustard seed as the test organism and three different concrete leachate concentrations revealed that the presence of PET plastic in concrete did not contribute to an increase in toxicity. Assessing both mechanical and ecotoxicological properties provides crucial information to anticipate potential long-term effects of such material in the future.

Keywords: concrete, ecotoxicity, ecotoxicological aspect, PET plastic waste

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Plasma-Assisted Chitosan Coatings on Cotton: Stability and the Challenges of Antimicrobial Assessment

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Functional textiles require durable antimicrobial finishes that withstand mechanical stress and repeated washing. Chitosan, known for its bioactivity, can be applied to cotton, yet the adhesion and long-term effectiveness are often insufficient [1]. This work investigates the durability of chitosan binding and antimicrobial potential following plasma-assisted surface modification.

Cotton fabrics were plasma-treated with low-pressure oxygen plasma (60 s) using a laboratory plasma reactor and impregnated with a 0.5 wt.% high molecular weight chitosan solution, which had been identified as optimal in our previous work [2]. Desorption studies were conducted by washing the samples and assessing chitosan retention through XPS and potentiometric titration. Plasma-activated samples retained more amino groups (R = 0.85) compared to untreated ones (R = 0.65), indicating improved coating stability.

Despite enhanced adhesion, antimicrobial testing against *Staphylococcus aureus* via agar diffusion revealed negligible inhibition zones for all treated samples. The strongest antimicrobial effect was anticipated for the sample treated with both plasma activation and chitosan impregnation. Compared to the untreated control sample, which showed dense bacterial growth around the textile, while the plasma-activated and chitosan-coated sample exhibited only a slight reduction in bacterial density—suggesting minimal but insufficient antimicrobial efficacy. This outcome is likely due to limited chitosan release under the tested conditions, possibly related to pH-dependent solubility. These findings underscore that the selected agar diffusion method proved inadequate for evaluating the antimicrobial efficacy of immobilized chitosan, as it failed to capture subtle non-leaching effects. However, this limitation itself is a valuable result, emphasizing the need for more suitable dynamic, contact-based assays in future studies targeting surface-bound biopolymers.

Overall, the results demonstrate that plasma activation enhances the durability of chitosan coatings, even though the antimicrobial effect is characterised as modest. Further improvements could include alternative coating strategies or surface design approaches that promote controlled bioactive release.

Key words: Chitosan, cotton fabric, antimicrobial textiles, plasma treatment, desorption, XPS, potentiometric titration.

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Bacterial cellulose-based anion exchange membranes for direct ethanol fuel cells

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Fuel cells (FCs) efficiently convert chemical energy into electrical energy and have a wide range of applications, but the high cost of components such as noble metals limits their commercialisation. Alkaline fuel cells (AFCs) with anion exchange membranes (AEMs) offer a cost-effective alternative as they can operate with non-precious metal catalysts. AFCs can also be fuelled with ethanol, referred to as direct ethanol fuel cells (DEFCs). Ethanol is an attractive alternative to the more toxic methanol and a supply chain already exists in many places. This type of FC is very promising as the supply and transport of the liquid fuel is much easier than gaseous hydrogen. It is also possible to use a biofuel (bioethanol) to ensure low CO_2 emissions or even CO_2 neutrality. However, current AEMs lack the performance required for commercial use in AFCs. Therefore, the development of efficient, environmentally friendly and affordable AEMs is crucial. [1] The synthesis of synthetic polymeric AEMs is usually complex, time-consuming and environmentally unfriendly. Natural materials such as chitosan, cellulose nanofibrils and bacterial cellulose (BC) are therefore attractive alternatives, especially as they can be readily modified. [2,3,4] Nevertheless, biopolymer-based AEMs still fall behind synthetic materials in terms of conductivity and strength, which can be improved by using suitable fillers and functionalisation techniques.

In our work, functionalized biopolymer BC-based membranes were investigated for their properties for use as AEMs in DEFCs. BC was functionalized with positively charged quaternary ammonium groups to improve the ion exchange capacity and ionic conductivity of native BC. Membrane properties investigated for the functionalized BC-based membranes included ethanol permeability, ion exchange capacity, swelling ratio, alkali uptake and ionic conductivity. A comparison was made with the commercial reference membrane Fumatech FAA-3-50. The data obtained indicate the applicability of the newly produced functionalized BC-based AEMs in DEFC technologies.

Acknowledgment: Financial support from the Slovenian Research and Innovation Agency is provided within the framework of the project “Efficient bacterial cellulose-based anion exchange membranes for alkaline fuel cell applications” (Z2-60175), “Nanofibrilar cellulose membranes in microbial fuel cells: material development for sustainable, high value-added applications” (J2-50086) and the Textile Chemistry and Advanced Textile Materials programme (P2-0118).

Keywords: bacterial cellulose, fuel cell, anion exchange membrane

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Raziskovanje znanstvenih in inženirskih konceptov z modelnim avtomobilom na gorivne celice

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Predstavljeni so rezultati raziskave znanstvenih in inženirskih konceptov zelene energije, ki smo jih izvedli v okviru NOO projekta ULTRA (Univerza v Ljubljani za trajnostni razvoj) na modelnem avtomobilu na gorivne celice. Oprema, ki smo jo uporabili, je vrhunsko orodje s strojno in programsko opremo in omogoča študijo zelene energije namenjeno študentom VSŠ Kemijske tehnologije. Spodbuja razvijanje novih rešitev za optimizacijo delovanja avtomobila, poučevanja področja opravljanja z energijo, raziskovanja razlik med pričakovanim delovanjem in eksperimentalnimi rezultati, raziskovanja delovanja gorivnih celic in odkrivanja kako doseči njihovo optimalno delovanje. S pomočjo tehnologije hibridnega pogona (gorivne celice in elektromotorja) in s pomočjo programske opreme modelni avtomobil omogoča razumevanje razlik vpliva na okolje glede na uporabljen pogonski agregat.

Oprema je bila kupljena v sklopu pilotnega projekta Trajnostni pristopi v kemijski tehnologiji katerega sofinancirata Republika Slovenija, Ministrstvo za izobraževanje, znanost in šport ter Evropska unija – NextGenerationEU. Ministrstvo za izobraževanje, znanost in šport je leta 2022 slovenske javne visokošolske zavode povabilo k oddaji vloge Pilotnega projekta VŠ UL za trajnostno družbo – ULTRA, ki je del Reforme visokega šolstva Mehanizma za okrevanje in odpornost, ki je namenjen prenovi visokega šolstva za zelen in odporen prehod.[1] Cilj pilotnega projekta je celovito naslavljanje in umeščanje kompetenc, ključnih za zeleni in digitalni prehod v učni načrt. Pri tem so bile upoštevane potrebe trga po znanjih in veščinah ter prestrukturiranju obstoječe in prihodnje delovne sile za oblikovanje Družbe 5.0 s koncepti vseživljenjskega učenja.[1] Študentje so z avtomobilom na gorivne celice pridobili vrhunsko opremo za laboratorijsko delo pri prenovljenem študijskem programu VSŠ Kemijska tehnologija.

SLIKA 1: Modelni avtomobil na gorivne celice

Rezultati pilotnega projekta bodo postali del kurikuluma VSŠ Kemijska tehnologija, s čimer bo študijski program postal modernejši in privlačnejši za bodoče generacije študentov.

REPUBLIKA SLOVENIJA MINISTRSTVO ZA VISOKO ŠOLSTVO, ZNANOST IN INOVACIJE | UNIVERZA V LJUBLJANI | NOO NAČRT ZA OKREVANJE IN ODPORNOST | Financira Evropska unija NextGenerationEU

SLIKA 2: Logotipi sodelujočih na projektu

Ključne besede: avto na gorivne celice, zelene tehnologije, praktično usposabljanje, digitalizacija

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SLOVENSKI KEMIJSKI DNEVI 2025

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A Comparative Study of Classical and Multiscale Modeling on Atropisomerism

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Methods based on molecular dynamics (MD) simulations are arguably the most rigorous approaches to calculating free energies and are ubiquitous in computational chemistry. Interactions in the studied systems can be described at several levels of sophistication and numerous approximations have to be made in practice [1]. While classical force fields [2] are sufficiently accurate for many applications, the fixed-point-charge approximation employed does not hold for highly polarizable systems. Quantum mechanical (QM) methods can be employed to address this limitation, however even semi-empirical approaches [3] remain too computationally expensive for most systems and simulation lengths desired. Multiscale QM/MM modeling [4, 5] poses an attractive alternative aiming to combine the best of both worlds – QM accuracy and force field efficiency.

Steric and electronic effects are among the most intricate to describe accurately in molecular simulations and pose a significant challenge. These phenomena can give rise to atropisomerism, a form of stereoisomerism due to hindered rotation about a bond and is particularly relevant in drug discovery [6]. In this study we assess the ability of classical and multiscale approaches to accurately capture stereoelectronic effects on a system of molecular balances [7]. We compare classical and QM/MM modeling as well as different enhanced sampling techniques. While all methods give free-energy differences within chemical accuracy, the obtained potentials of mean force differ significantly. Barrier heights vary, and more surprisingly, the identified local minima are shifted notably. Detailed analysis of these observations is carried out, factors leading up to these effects are investigated and practical implications for prospective applications are discussed.

Keywords: free-energy calculations, multiscale QM/MM modeling, stereoelectronic effects, atropisomerism

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Molecularly imprinted polymer-based strategy for electrochemical detection of acetamiprid

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Acetamiprid (ACM), a widely used neonicotinoid insecticide, is frequently present in surface waters and agricultural products, raising concerns due to its potential neurotoxic effects on non-target organisms, including pollinators and humans. Effective monitoring of ACM requires development of sensitive, fast, and reliable detection methods [1]. Electrochemical techniques offer a rapid and low-cost alternative to conventional chromatographic methods (e.g. LC-MS), combining portability, fast response, and operational simplicity, which makes them particularly well-suited for on-site analysis [2]. However, direct electrochemical detection of ACM is not feasible due to its electrochemical inactivity within the potential window of carbon-based working electrodes (WE). To overcome this limitation, a molecularly imprinted polymer (MIP) has been synthesized and applied as a selective recognition element on the WE surface, enabling indirect voltammetric detection based on current suppression of a redox probe.

Key parameters for bulk MIP synthesis, including monomer type, solvent, prepolymerization conditions, and reagent ratios, were systematically optimized to obtain a material with high affinity and selectivity toward ACM. The best-performing MIP with an imprinting factor of 2.12 and a binding capacity of 7.14 µmol/g was selected for further characterization. Adsorption behaviour of ACM was consistent with the Langmuir–Freundlich binding isotherm and pseudo-second-order kinetics. MIP was subsequently used to modify the WE for indirect ACM detection, based on current suppression of the redox probe (hexacyanoferrate(III)/hexacyanoferrate(II), HCF) after WE incubation in the analyte solution. Preliminary characterization was performed using cyclic voltammetry on screen-printed carbon electrodes, as well as on a conventional three-electrode system employing a glassy carbon electrode (GCE). The most pronounced decrease in anodic peak current in 5 mM HCF was observed after a two-layer drop-casted modification of the GCE using a 5 mg/mL MIP suspension. Selectivity was confirmed in the presence of structurally related neonicotinoids. Scan rate studies indicated a reduced electroactive surface area of the WE after ACM binding, consistent with the observed signal suppression. Quantification by differential pulse voltammetry in the 1–100 µM concentration range showed good linearity between the current change (Δi) and log$c$ (R^2 = 0.989) corresponding to calculated limit of detection (LOD) of 1.06 µM. This approach combines molecular selectivity with the practical advantages of electrochemical analysis, offering a promising platform for the detection of neonicotinoids. Further work will focus on improving the LOD by incorporating conductive nanomaterials and optimizing the MIP particle size, as well as adapting the method for screen-printed electrodes to enable portable and field-deployable sensing.

Keywords: Neonicotinoids, acetamiprid, molecularly imprinted polymer, drop-casting, indirect electrochemical detection

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Precise determination of Cd isotope ratios in a candidate reference seawater material

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The accurate and precise isotope ratio determination is of strong interest to many researchers due to its implications in earth, environmental, biological, medical, and archaeological sciences. Due to the development of mass spectrometry techniques, it is possible to detect small differences in the isotope composition of elements. Multicollector inductively coupled plasma mass spectrometry (MC ICP-MS) is a user-friendly and efficient method for obtaining high-precision isotopic data – it enables the determination of isotope ratios with a measurement precision down to 0.001 % [1].

Cadmium (Cd) is a naturally occurring element, with eight stable isotopes ^{106}Cd, ^{108}Cd, ^{110}Cd, ^{111}Cd, ^{112}Cd, ^{113}Cd, ^{114}Cd, and ^{116}Cd. Accurate determination of Cd isotope ratios provides valuable insights across broad range of disciplines, including cosmochemistry, geochemistry, and environmental sciences, as they can be used to trace pollution sources, study biogeochemical cycles, and asses isotope fractionation processes. Of particular interest is the role of Cd in oceanic biogeochemical cycles, as Cd undergoes fractionation during assimilation into biological material. Despite their significance, the challenges in using Cd isotopes in analytical and environmental research lie in the lack of available isotope certified reference materials (CRMs). This scarcity hinders the standardization of isotope ratio measurements, limiting consistency and inter-laboratory comparability of analytical results. Additional challenge in precisely determining Cd in seawater, despite big instrumental advancements, is due to low Cd concentrations in a complex, high-salinity matrix. That is why a high-quality sample pre-treatment is necessary – Cd must be completely separated from the matrix and any interfering elements. Commonly applied methods for matrix separation or preconcentration of Cd involve coprecipitation and solid phase extraction [2,3].

The aim of the study was to characterize and precisely determine the Cd isotope composition of a candidate reference seawater material. For that, the methods for triethylamine-assisted $Mg(OH)_2$ coprecipitation and Cd separation on a column, filled with an ion-exchange resin AG-MP-1M, were implemented and optimized. The mass balance through all the steps was followed by measuring the total Cd concentration with ICP-MS. Cd isotope ratios were determined with MC ICP-MS. The results showed that both methods were suitable for determining Cd isotope composition in seawater matrix, as there was no loss in total Cd concentration, the removal of interfering elements was sufficient, and no fractionation of Cd occurred during the preparation process.

Keywords: Cd isotopes, heavy matrix, sea water, coprecipitation, column separation

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Determination of *in vitro* antioxidant activity of Himalayan balsam (*Impatiens glandulifera* Royle) extracts based on three different extraction techniques

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Himalayan balsam (HB) is spreading extremely rapidly across Europe – with an annual expansion rate of approximately 645 km², it is regarded as one of the most invasive alien plant species. As an annual plant, it primarily thrives near watercourses, where it successfully displaces native vegetation by exploiting available resources and through allelopathic interactions. Due to its widespread occurrence and ecological impact, there is increasing interest in identifying meaningful ways to utilize this species, such as for medicinal purposes [1].

The choice of an appropriate extraction technique plays a crucial role in the efficiency and yield of biologically active compounds from plant materials. Different methods affect the composition and stability of the obtained extracts, as they utilize various mechanisms for releasing compounds from plant matrices. In addition to the extraction method, the selection of a suitable solvent is also essential for successful extraction. Bioactive components vary in their polarity, which means the solvent must be tailored to the target group of compounds. Optimal extraction therefore requires a carefully coordinated choice of both method and solvent, as an inappropriate combination may result in low yields, poor selectivity, or degradation of sensitive compounds [2].

It has been repeatedly noted that HB contains compounds that attract interest in both scientific and industrial fields. Due to the presence of bioactive constituents, extracts from *Impatiens* species are increasingly being considered as a potential source of natural antioxidants [3].

This study reports on the *in vitro* antioxidant activity of whole-plant extracts of HB, obtained using a combination of two solvents (methanol and *n*-heptane) at three extraction temperatures (30 °C, 45 °C, and 60 °C), while employing three extraction techniques: maceration, ultrasound-assisted extraction, and accelerated solvent extraction. The samples were analysed by using two complementary spectrophotometric *in vitro* antioxidant assays based on free radical neutralization: 2,2-diphenyl-1-picrylhydrazyl (DPPH) and 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS).

Keywords: Himalayan balsam, extraction technique, extraction solvent, antioxidant activity.

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Connecting hydrogen bonding and resonance frequency of water in alternating electric field

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Nowadays, we are surrounded by electromagnetic radiation of different wavelengths, which also influences the properties of molecules. When it comes to the interaction of an electromagnetic field with molecules, most of the effect comes from the electric component of the field, while the magnetic component can be negligible. Here we have investigated how an alternating electric field with different frequencies influences the properties of rose water model[1]. Rose water model is a simple two-dimensional water model in which the molecules are represented as Lennard-Jones discs with explicit hydrogen bonding potential. The model also has partial charges that enable the interaction between the molecules and the electric field. The alternating electric field affects all properties of the water model, with the effects of the field depending strongly on the amplitude and frequency of the field.

The focus of this study was on the electric field in the microwave region, where the frequency of the electric field is in the range of the rotational motion of the (water) molecules. Depending on the strength of the electric field, three different regimes of electric field effects are observed. If the frequency of the field coincides with the frequency of the rotational motion, resonance occurs. The resonance frequency depends on the environment of the individual water molecules (their hydrogen bonds) and the strength of the electric field. We have developed a simple model that predicts the rotational absorption spectra of water in an electric field based on the statistics of the hydrogen bonds. The model uses populations of nonbonded and bonded water molecules, each population having its own resonance frequency. The resonant frequencies of the populations depend on the average number of hydrogen bonds in the system and on the strength of the electric field. In addition to the model that predicts the rotational absorption spectra of water, we have also developed a simpler model that predicts the resonance frequency of water in an alternating electric field of varying strength. Both models establish the relationship between the hydrogen bonding of the water molecules and their rotational spectra or resonance frequencies in the electric field. These models could also be used for experimental measurements where the hydrogen bonding statistics of the water molecules could be calculated from the resonance frequency in the electric field.

Keywords: water model, electric field, resonance, hydrogen bonding

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Influence of ion-specific effects on structural properties of polyelectrolyte solutions

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Polyelectrolytes are a subtype of linear polymers with charged monomer units. Ionenes, a specific class of polyelectrolytes, consist of alkyl chains with varying lengths of methylene groups, interspersed with positively charged quaternary nitrogen atoms. Ionenes are classified as x,y-ionenes, where x and y indicate the number of methylene groups separating adjacent nitrogen atoms (e.g., 3,3-ionene). With increasing length of hydrophobic alkyl chains between nitrogen atoms, charge-density of ionene decreases [1,2]. The term "ion-specific effects" refers to changes in the properties of polyelectrolyte solutions that are influenced by a change in charge-density of the ionene and/or its halide counter-ions [3]. These effects are fundamental in numerous biological processes, including membrane transport, osmotic regulation, and enzymatic activity, and they also significantly impact the structure and function of proteins, phospholipids, nucleic acids, and polysaccharides [4]. In our work, ion-specific effects in four different systems with varying charge-density of the ionene (3,3-/6,6-ionene) and counter-ions (F^-/Br^-) were investigated. By employing high and low charge-density species for both ionene and counter-ions, we investigated ion-specific effects of both simple and polyions, as well as their impact on structural phenomena in aqueous solutions. Molecular dynamics (MD) simulations of all systems were performed at 298K and 1bar in OPLS-AA force field. Water was modelled explicilty by using the SPC/E water model. From MD simulations we calculated radial distribution functions (RDF) between various structural domains in each of the four systems. The results revealed that Br^- ions exhibit higher probability of being in close proximity (or even condensing) to either type of ionene compared to F^- ions. Br^- ions have, due to their chaotropic nature, loosely bound 1st hydration shells and are capable of losing 1-2 water molecules when condensing on the ionene chain (often around charged nitrogens). In contrast, kosmotropic F^- ions maintain tight and compact hydration shells, which always remain largely intact, resulting in them staying further away from the ionene molecules. We conclude that Br^- ions condense on both 3,3- and 6,6-ionene, mostly on charged nitrogens or their neighbouring groups. In the case of F^- ions, condensation sometimes occurs on the methyl(ene) groups of the 3,3-ionene. Our findings are in agreement with past experimental results [5].

Keywords: polyelectrolytes, ion-specific effects, charge-density, radial distribution function

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Synthesis and photochemical transformations of novel pyridazinone derivatives

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In recent years, pyridazinone derivatives have emerged as an important class of compounds in medicinal chemistry due to their diverse and potent biological activities. Although originally developed for cardiovascular and agrochemical applications, pyridazinones have since demonstrated a broad spectrum of pharmacological properties, including antimicrobial, anti-inflammatory, antidiabetic, anticancer and antifungal activities. [1,2] When embedded in a fused bicyclic pyrazolopyridazinone system, these compounds show promising potential as enzyme inhibitors, such as BTK kinase inhibitors. [3] While some pyrazolopyridazinone derivatives are readily accessible via multicomponent synthetic strategies, others remain challenging to obtain.

In this work, we report a novel one-pot synthetic route to pyrazolo[1,2-*a*]pyridazinones, characterized by mild reaction conditions and high atom economy. Due to their strong absorption in the visible light range, we investigated the potential of these compounds for direct photochemical functionalization. By tuning the reaction conditions, we successfully prepared a variety of structurally diverse pyridazinone derivatives from pyrazolo[1,2-*a*]pyridazinones without the use of external (photo)catalysts. These light-induced transformations proceed rapidly, exhibit high atom economy, and allow the formation of sterically challenging scaffolds that are difficult to access using conventional synthetic methods.

The developed approach is operationally simple, environmentally friendly, compatible with a wide range of functional groups and provides a valuable platform for the efficient synthesis of biologically relevant pyridazinone-based scaffolds.

Keywords: pyridazinones, photochemical transformations, one-pot synthesis, atom economy.

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Transition Metal-Free Deuteration of Heteroaryl *O*-Carbamates and Carboxamides Using Directed *ortho*-Metalation

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Compounds containing deuterated *N*-heterocycles have been used to improve the efficacy by modulating their metabolism[1] and found applications as functional materials with improved stability and performance compared to their non-labelled counterparts.[2] The development of approaches for selective deuteration of *N*-containing heterocycles is highly coveted but largely reliant on Transition metal catalysts which are expensive and difficult to recycle.[3] Research on some alternative approaches has been reported (e.g. using electrochemistry[4]) but is limited by modest D-incorporation and poor site selectivity. Another approach that has been explored involves the use of Directed *ortho*-metalation (DoM), followed by quench with an electrophilic source of deuterium.[5] Although a lot of work has been done on DoM-deuteration over the years, deuteration of electron-deficient heteroaromatic systems remains relatively unexplored.[6]

Here we report the site-selective H/D exchange of heteroaromatic compounds functionalized with an *O*-carbamate or a carboxamide group as a directing group (DG) (**Figure 1**). H/D exchange was performed using organolithium bases and D_2O as a safe and relatively inexpensive source of electrophilic D^+. The products were obtained with good chemoselectivity and D incorporation.

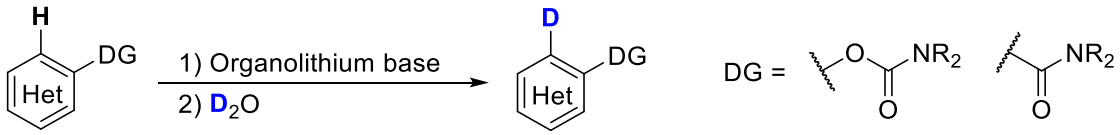

Figure 1: *Site-selective deuteration of heteroaromatic compounds using O-carbamate and carboxamide as a DG.*

Keywords: Deuteration, *O*-carbamate, carboxamide, heteroaryl, directing group

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Functionalized 1,3-dialkylimidazolium ionic liquids: thermodynamic models of mixing with water

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Ionic liquids (ILs) are salts with melting points below 100 °C. Due to their promising potential for application in areas such as electrochemistry and organic synthesis [1,2], as well as the ease of their synthesis, imidazolium compounds have so far been among the most studied classes of ionic liquids. While most commonly their cations contain long alkyl chains, the inclusion of specialized functional groups into those chains is often possible. Such compounds have previously been used to facilitate the absorption of CO_2 from air [3], and in the preparation of various types of nanomaterials [4]. All ionic liquids also have a very high affinity for atmospheric water; therefore the study of the thermodynamics of their mixtures with water is of paramount importance.

Several 1-alkyl-3-methylimidazolium acetate ionic liquids have been synthesized from their bromide precursors via ion-exchange. In all instances, the alkyl chain consisted of two methylene groups, and a functional group (hydroxyl, amine or carboxylic). The densities, viscosities and refractive indices were measured for the pure ionic liquids. Water was then titrated in small aliquots (4-5 μL) into the prepared compounds with TAM IV calorimeter (TA Instruments, New Castle, USA) at different temperatures. The enthalpies of mixing with water were then obtained with respect to the composition in the sample cell. PC-SAFT (*perturbed-chain statistical associating fluid theory*) equation of state was used to fit the experimental data to obtain the model parameters for ionic liquids. Standard association schemes were used for used for water, while the ionic liquids were described as neutral molecules, using multiple-site association schemes.

In the future, ePC-SAFT (electrolyte PC-SAFT) theory will be used to incorporate electrostatic interactions explicitly and improve upon the existing model by allowing for a better description of hydrogen bonding with water.

Keywords: ionic liquids, model, electrolyte, equilibrium

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Synthesis of Substituted Carbazoles for Optoelectronic Applications

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Carbazole-based molecules are widely used as hole-transporting self-assembled monolayers (SAMs) in p-i-n perovskite solar cells (PSCs) (Scheme 1) due to their favorable optoelectronic properties, synthetic tunability, as well as their thermal and morphological stability.[1,2] The properties of PSCs are closely related to the structure of SAMs, which is why precise control over molecular orientation, electronic structure, and anchoring group design is essential to enable efficient hole transport, long-term indium tin oxide (ITO) stability and achieve optimal alignment of SAMs HOMO and electrode work function (WF).[2,3] While many studies have focused on horizontal carbazole architectures,[3] less is known about the impact of orientation and dipole alignment at the molecular level. In this study, we explore structure–property relationships of vertically aligned carbazole SAMs. We used calculated HOMO energies and dipole moments of various derivatives to guide the structural tuning of the SAMs.

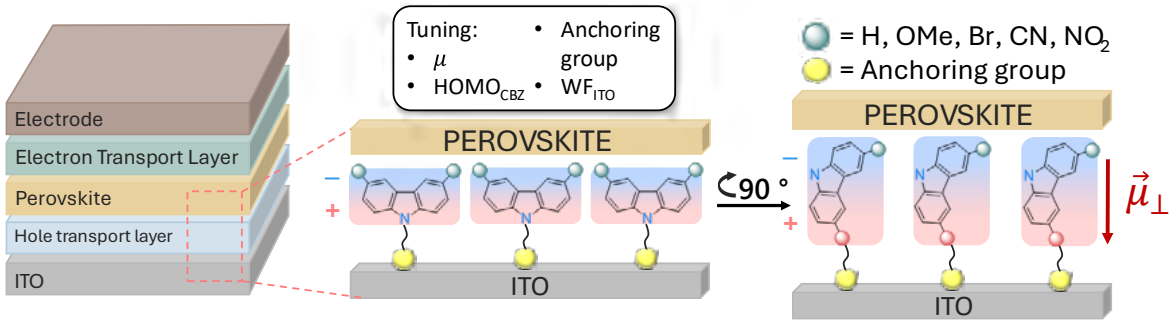

Figure 1: Schematic representation of a p-i-n perovskite solar cell and SAM interface tuning. Carbazole molecules are flipped by 90 ° adopting a vertical orientation resulting in an increased dipole moment

We will present our strategy for rational molecular design via 90 ° carbazole orientation (Scheme 1) and analyze how parameters such as HOMO, dipole and anchoring groups affect the properties of PSCs. Anchoring groups including phosphonic acid, boronic acid and carboxylic acid will be compared in terms of work function modulation, ITO compatibility, and long-term stability. This combined computational–experimental approach allows for the systematic optimization of carbazole-based interlayers in next-generation optoelectronic devices.

Keywords: tandem solar cells, SAMs, carbazoles, dipole moment

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Synthesis of Serine-Based Fluoroalkyl Ethers as Sensitive ^{19}F NMR Reporters *via* the Mitsunobu Reaction

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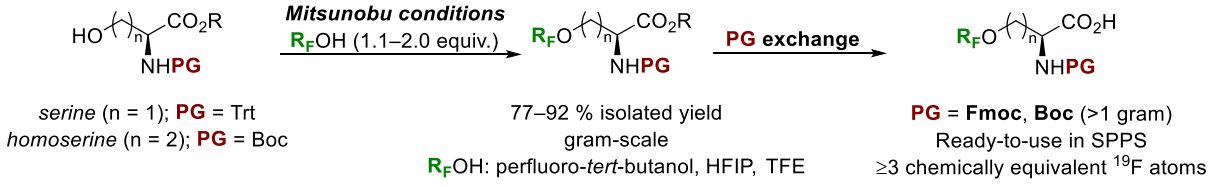
Peptides are a promising therapeutic modality that combine the advantages of biologics and small molecules [1]. However, their clinical utility is limited by poor cell permeability, low *in vivo* stability, and limited oral availability [1]. Incorporation of unnatural amino acids (AAs) is a key strategy of structural modification to overcome these pharmacokinetic limitations [2]. In particular, the incorporation of fluorine-containing AAs has been shown to improve metabolic stability and cell uptake, enhance hydrophobicity, stabilize specific secondary structures, and enable investigation of peptide–protein interactions *via* ^{19}F NMR spectroscopy [3].

The development of sensitive, fluorinated AA-based ^{19}F NMR reporters that can be readily incorporated into bioactive peptides is crucial for advancing our understanding of biochemical interactions [4]. However, the majority of available fluorinated AAs feature no more than three chemically equivalent fluorine atoms, often coupled to other nuclei, which leads to complex NMR coupling patterns and reduced sensitivity. The Mitsunobu reaction with fluorinated alcohols as nucleophiles represents an underexplored approach for introducing fluoroalkoxy groups bearing multiple chemically equivalent fluorine atoms into hydroxyl-containing AAs.

Herein, we present the development of fluorinated serine derivatives using the Mitsunobu reaction with various fluorinated alcohols. The synthesis of perfluoro-*tert*-butyl serine derivatives was optimized and efficiently carried out on a gram scale. Subsequent protecting group exchange afforded *N*-Boc and *N*-Fmoc protected building blocks in high overall yield, suitable for both solution-phase and solid-phase peptide synthesis. Additionally, alternative fluorinated alcohols such as HFIP and TFE were explored as Mitsunobu nucleophiles.



Keywords: Organofluorine chemistry, Unnatural amino acids, ^{19}F NMR spectroscopy, Mitsunobu reaction.

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From Cellulose to Value-Added Chemicals: Oxidation Reactions and Platform Molecules Synthesis

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The transition from a fossil-based to a bio-based economy requires the development of sustainable and renewable sources of chemicals, fuels and materials. The utilisation of surplus biomass (e.g. plant residues that cannot be used as food), which is sometimes thrown away or even incinerated, plays an important role in this transition. Lignocellulosic biomass, which consists mainly of cellulose, hemicellulose and lignin, has emerged as a promising alternative feedstock due to its carbon neutrality.[1] Among these components, cellulose is particularly attractive due to its large natural abundance, structural uniformity and potential for targeted chemical conversion into useful chemicals and materials.

Cellulose is the most abundant polymeric material in nature. It is a linear polymer of β-D-glucopyranose units linked by β(1→4) glycosidic bonds that assemble into crystalline microfibrils. This organised structure provides the mechanical strength of plant cell walls and offers both opportunities and challenges for isolation and chemical processing.[2] While crystallinity can limit reactivity, the surface of the polymer is rich in hydroxyl groups, providing numerous sites for selective functionalisation and chemical refinement, e.g. by etherification, esterification, sulphonation, amination, etc. reactions. In addition, its structure also enables oxidation reactions.

The oxidation of cellulose opens the way to a wide range of high-quality compounds. Two main processes can take place during the oxidation of cellulose, namely the oxidation of hydroxyl groups on the cellulose chain or the oxidative cleavage of β(1→4) glycoside bonds. This produces molecules such as 5-hydroxymethylfurfural (HMF) and 2,5-furandicarboxylic acid (FDCA), which are starting materials for bio-based polymers (e.g. PEF or PET).[3] Other oxidation products, including acids and related compounds, are used as biodegradable solvents or chemicals and in the food, pharmaceutical or cleaning industries.

In our work we investigate different possibilities of cellulose isolation and their effects on the yield of the delignification reaction and on the morphological properties of the isolated cellulose. We have further investigated the selective oxidation of cellulose and direct oxidation of biomass, which leads to the disruption of the aromatic structure of lignin and to the isolation of the oxidised form of cellulose. Our results contribute to a more comprehensive understanding of cellulose oxidation chemistry and support the development of innovative and sustainable processes for biomass utilisation.

Keywords: lignocellulosic biomass, cellulose, monosaccharides, oxidation, platform molecules.

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Site-specific introduction of alkyne-functionalized unnatural amino acid into recombinant protein targets *in vivo*

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The field of protein bioconjugation has unlocked the ability to covalently attach proteins to a diverse array of molecules, including fluorescent tags or even other biomolecules, facilitating advances in targeted drug delivery, immobilization and precise biomolecular labelling. Achieving greater specificity in these conjugation strategies necessitates the development of novel chemo selective methods to forge unique covalent linkages between biomolecules. Terminal alkynes serve as valuable biorthogonal handles, as they are absent from natural proteins yet readily participate in a variety of selective, bioorthogonal reactions, such as Glaser coupling, Sonogashira coupling, the thiol-yne reaction and most notably the copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC), a hallmark of "click" chemistry.

In this work, we focused on the *in vivo* incorporation of the alkyne-functionalized noncanonical amino acid 4-propargyloxy-L-phenylalanine (pPrF) into two novel protein constructs by employing amber stop codon (TAG) suppression in *Escherichia coli*, utilizing a tailored orthogonal aminoacyl-tRNA synthetase (aaRS)/tRNA system. Following purification via His-tag affinity chromatography, we successfully produced two proteins each bearing a single alkyne group: the bleomycin resistance protein (BRP) from *Streptoalloteichus hindustanus* at residue Y75, and the N-terminal domain of the ribosome maturation factor RimM from *Thermus thermophilus* at residue Y34. Incorporation was verified by liquid chromatography-mass spectrometry (LC-MS), whilst we used CD spectroscopy to confirm the same secondary structures in both modified and unmodified proteins.

Owing to its efficient pPrF incorporation, compact structure, thermostability, robustness, minimal steric impact, and suitability for generating homogenous protein conjugates, RimM Y34-pPrF emerges as an excellent candidate for future investigations into alkyne-based bioorthogonal reactions and their kinetic properties.

Keywords: terminal alkynes, bioorthogonal chemistry, unnatural amino acids, site-specific modifications, amber codon suppression

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Towards strategies for incorporating non-natural fragments into polypeptides and their synthesis in aqueous solution

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In recent years, peptides have become increasingly prominent across various fields of science, both in academic research and industrial applications. As a result, the demand for modified and customized peptide variants continues to grow. The most commonly used method for the preparation of peptides (and smaller proteins) through chemical synthesis, is by using solid-phase peptide synthesis (SPPS). The process operates under heterogeneous conditions on a polymeric solid support and is based on complementary protective groups and reactions that are designed to achieve nearly quantitative conversions. SPPS proceeds through a step-by-step process where activated amino acids are sequentially added to a growing peptide chain to enable complete control over amino acid sequence. After each coupling step, the protective group, typically Fmoc, is removed from the amine group of the last amino acid in the chain, allowing it to react with the carboxyl group of the next amino acid. Throughout the synthesis, excess reagents and byproducts are washed away using organic solvents, most commonly N,N-dimethylformamide (DMF). Despite being a costly method due to the high consumption of expensive supports, amino acids, solvents, and coupling agents, SPPS remains widely used, also in industry [1].

Further, these polypeptide structures can be further modified by introducing unnatural amino acids bearing desired fragments. To this end the established SPPS, a process that has been increasingly automated in recent years, can also be used [2]. In our work, we have synthesized a modified phenylalanine derivative bearing an azide group at the para-position of the aromatic ring. This type of amino acid is particularly valuable because it can participate in well-established reactions, such as copper-catalyzed azide-alkyne cycloaddition.

Despite these advances, one of the key goals is to develop more sustainable peptide synthesis approaches, which would allow the use of natural unprotected amino acids, simple activators, and green solvents, such as water. We attempted such a synthesis through optimizing the preparation of a dimer between 3-phenylpropanoic acid and L-alanine, which served as model substrates. These optimizations will be discussed as well as results of integrating the above described non-natural fragments structures into biomolecules, such as peptides and proteins, where aim is to investigate how such structural modifications influence their overall conformation and biological activity.

Keywords: solid-phase peptide synthesis (SPPS), polypeptides, unnatural amino acids, azide functional group

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Synthesis and Structural Evaluation of Iron-Zinc Double Metal Cyanides complex: Effect of complexing and co-complexing agents

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Double metal cyanides (DMCs) are coordination polymers consisting of two different metal centers bonded by a cyanide group. They are well-known catalysts for the copolymerization of epoxides and CO2, enabling the production of biodegradable polycarbonates [1,2]. Additionally, they are used in the synthesis of propylene oxide-based polyether polyols, which are widely employed in various polyurethane applications. This study provides insight on structural characterization of Fe-Zn DMC prepared from the aqueous solutions of Zinc chloride (ZnCl2) and potassium hexacyanoferrate (K4Fe(CN)6) in the presence of tert-butanol (complexing agent) and triblock copolymer (co-complexing agent) [2]. A series of DMC were prepared with and without complexing and co-complexing agents. Synthesized catalysts were analyzed by different techniques such as Infrared spectroscopy, BET surface area, Raman spectroscopy, scanning electron microscopy (SEM), and X-ray diffraction (XRD) to determine the structural variations in the catalysts.

The results indicate that both the crystal structure and the electron-donating nature of the complexing agent significantly influence the catalytic activity and selectivity of the DMCs. Notably, DMC samples prepared with both complexing and co-complexing agents exhibited higher acidity, which was directly correlated with enhanced catalytic performance.

Keywords: Iron-Zinc cyanide complexes; Interfaces; Effect of complexing agent; synthesis method, Surface area

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Coordinating something new

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Humans have been fighting microbes for centuries, initially using metal-based remedies such as silver, arsenic and mercury salts with varying results. The discovery of antibiotics at the beginning of the 20th century changed the treatment of infections and saved millions of lives. However, their overuse has led to the development of antimicrobial resistance, which is recognized by the World Health Organization as a serious threat to public health. To counter this, efforts are focusing on smarter use of antibiotics, improving existing drugs and exploring innovative solutions such as metal-based compounds [1].

In the 1950s, a potential new compound was discovered while studying an extract of *Streptomyces caerules*. The researchers noticed that something in this extract inhibited the growth of various filamentous fungi, yeasts and some bacteria. After isolation and characterization, they discovered a novel asymmetric 2,2'-bipyridine, which they named caerulomycin, later named caerulomycin A (CaeA) (**Figure 1**) [2]. Further research has shown that these compounds not only have antifungal and antibacterial activity, but also exhibit anticancer, immunoregulatory and other potential therapeutic properties [2–4].

The first synthesis of CaeA was achieved in 1969. Later, in 1998, a route to produce CaeE, a precursor convertible to CaeA, was developed [5]. We succeeded in optimizing and improving the yield of this synthesis on a gram scale in combination with newer published procedures [6]. With the synthesized CaeE, we successfully prepared the first rhenium complex containing CaeE as a ligand.

Keywords: metal complexes, coordination chemistry, caerulomycin

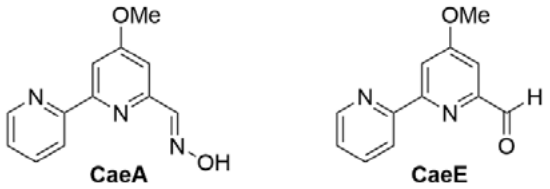

Figure 1: Structure of two Caerulomycins

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Funding information: We are grateful for the financial support from the junior research grant for Jure Jakoš and program grant P1-0175 of the Slovenian Research and Innovation Agency (ARIS). The authors also acknowledge the support of the Centre for Research Infrastructure at the University of Ljubljana, Faculty of Chemistry and Chemical Technology, which is part of the Network of Research and Infrastructural Canters UL (MRIC UL) and is financially supported by ARIS; Infrastructure program No. I0-0022.

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Influence of Defect Chemistry on the Electrochemical Performance of Li-rich Oxides

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Li-rich layered oxides (LROs) are considered among the most promising high-voltage cathode materials for improving the efficiency of lithium-ion batteries (LIBs), owing to their low toxicity and cost-effectiveness. These materials have demonstrated capacities that exceed those of conventional cathode materials such as $LiCoO_2$ [1]. However, their widespread application is hindered by persistent challenges, including low initial coulombic efficiency, voltage decay, and limited high-rate performance[2], challenges rooted in their structurally complex nature.

In this study, we synthesized $Li_{1.2}Mn_{0.54}Co_{0.13}Ni_{0.13}O_2$ using a sol-gel method, varying the chelating agent (citric vs. oxalic acid) and calcination temperature (850 °C and 900 °C) to study their influence on structure and performance. XRD analysis revealed that oxalic acid, being a less effective chelating agent, produced a more disordered structure with pronounced stacking faults and oxygen vacancies. EELS measurements further indicated a higher presence of Mn^{2+} species in these samples, consistent with increased oxygen deficiency.

Despite the higher degree of disorder, oxalic-acid-derived LROs exhibited improved electrochemical performance across both temperatures. Operando XRD showed that these samples maintained a larger unit cell volume after discharge, a feature that may help suppress Li/Ni intermixing and spinel phase formation, key factors in long-term cycling stability.

Overall, our findings suggest that controlled introduction of structural defects through synthesis tuning can enhance LRO performance. This highlights defect engineering as a valuable strategy for optimizing cathode materials in next-generation energy storage applications.

Keywords: Li-rich layered oxides, oxygen vacancies, stacking faults, sol-gel synthesis, lithium-ion batteries

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Probing the Impact of Mass Transport on Meniscus Electrochemistry by Time-Resolved Operando X-ray Photoelectron Spectroscopy

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Ambient pressure X-ray photoelectron spectroscopy (APXPS) combined with the dip-and-pull method has been thought of as a method particularly suitable for operando studies of electrochemical systems. APXPS probes the electrode/electrolyte interface through the meniscus, whereas electrochemistry collects signals from the meniscus and in bulk electrolyte. Mass transport in the meniscus is not the same as in the bulk electrolyte and the exact impact of mass transport differences on the meniscus electrochemistry is unknown. The difference between the meniscus and the bulk electrolyte mass transport and its impact on the meniscus mass transport are systematically investigated in this work by simultaneously conducting time-resolved APXPS and chronoamperometry for two types of electrochemical processes: capacitive and faradaic. Experiments are conducted on a model system consisting of a gold electrode and carbonate electrolyte. Moreover, experiments are complemented with simulations based on a purposefully constructed transmission line model. A significant meniscus resistance is observed and the ensuing iR drop is shown to have a large influence on the meniscus electrochemistry. Specifically, the large iR drop during faradaic processes results in two to three orders of magnitude slower rate of faradaic processes in the meniscus as opposed to the bulk electrolyte. Based on the gained understanding of the meniscus electrochemistry, we suggest an experimental practice to quantify the iR drop and propose possible remedies for experiments where any impact of the iR drop must be avoided.[1]

Keywords: mass transport limitations, dip-and-pull, electrochemistry, interfaces, ambient pressure

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Organic cathode materials for diverse battery applications

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The large-scale deployment of battery technology is driving the research towards the use of more sustainable and less scarce materials. In recent years an alternative to the presently used inorganic cathode materials has emerged in the form of organic cathode materials, which can be made out of abundant raw materials with a lower carbon footprint. Since the traditional inorganic lithium-ion-battery cathodes are reaching their upper theoretical limitations and the room for discovering new intercalation materials is narrow, an alternative pathway of using organic materials could present a future breakthrough in achieving higher energy density and more sustainable post lithium-ion batteries.

The presentation will detail our results concerning the development of novel organic cathode materials. The materials are based on quinone and pyrazine redox-active units and are intended for application in lithium and zinc batteries [1,2,3]. We will discuss their synthesis strategies, which also utilize biomass-derived precursors. Performance metrics will be presented, highlighting active material energy densities reaching up to 860 Wh/kg in lithium batteries and 330 Wh/kg in zinc batteries, figures that represent significant advancements in the field. Furthermore, we will provide an in-depth analysis of the underlying redox mechanisms inherent to these materials.

Keywords: batteries, organic cathode, zinc, lithium, zinc

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Key role of surface chemistry in thermodynamic stability of two-dimensional transition metal carbides/nitrides (MXenes)

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Two-dimensional transition metal carbides and nitrides (MXenes) have been reported as promising materials for various applications, including including energy generation and storage, catalysis, healthcare, photonics, and electronics [1]. The family of MXenes has proliferated, and the chemical space of synthesized MXenes has expanded to 13 transition metals and a dozen elements in surface terminations [2]. The diverse chemistry of MXenes enables systematical tuning of MXene properties to meet the needs of target applications. However, synthesizing new MXene compositions largely relies on a trial-and-error approach. To overcome it, computational predictions of MXene compositions that are thermodynamically stable are crucial to rationalize experimental efforts [3].

We performed a comprehensive density functional theory (DFT) screening for thermodynamically stable MXenes across 29 transition metals and 11 surface terminations to elucidate factors affecting their thermodynamic stability and identify stable MXene compositions [4]. We have combined the database DFT data to construct 638 compositional phase diagrams and performed high-throughput DFT calculations of 7888 MXene structures as well as 687 thermodynamically competing phases to assess the thermodynamic stability of the MXene family. The pivotal role of the surface termination chemistry in the overall thermodynamic stability of MXenes has been shown, and many new (meta)stable MXene compositions across the wide MXene chemical space have been identified, laying the foundation for MXene genomics (materials genomics of MXenes).

Keywords: MXene, thermodynamics, surface termination, density functional theory, materials genome

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Enhancing Recycled Nd–Fe–B Magnets: Grain Boundary Control with Multicomponent Alloy Additions

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The pursuit of high-performance, sustainable Nd–Fe–B magnets has shifted focus toward recycling, reduced use of heavy rare earths, and microstructural optimization. Despite excellent properties, commercial magnets utilize only ~20% of their theoretical coercivity due to inadequate grain boundary phases [1]. This challenge intensifies in recycled powders from Hydrogen Processing of Magnetic Scrap (HPMS), where oxidation and Nd-phase loss degrade performance [2]. In this study, HPMS-derived powders were selectively leached to yield single-phase $RE_2Fe_{14}B$ material. A bottom-up microstructure redesign strategy was then applied, incorporating low-eutectic alloys to improve densification during sintering, refine grain boundary chemistry, and enhance the magnetic properties of upcycled magnets. Single-phase $RE_2Fe_{14}B$ powder was consolidated through Spark Plasma Sintering (SPS) using 10 wt% additions of various low-melting alloys: $Nd_{70}Cu_{30}$, $Nd_{33}Cu_{67}$, $Nd_{48}Ce_{32}Cu_{20}$, $Nd_{50}Tb_{20}Cu_{30}$, and $Nd_{50}Dy_{20}Cu_{30}$. To a varying degree, these acted as liquid-phase sintering aids and GB modifiers, promoting improved densification and magnetic decoupling. The best performance was achieved with $Nd_{50}Tb_{20}Cu_{30}$ alloy, reaching coercivity values above 1500 kA/m. Using $Nd_{50}Tb_{20}Cu_{30}$ and $Nd_{33}Cu_{67}$ alloys represent complementary design strategies: performance optimization and material efficiency, respectively. Powder blends incorporating them were selected for more in-depth investigation. For $Nd_{50}Tb_{20}Cu_{30}$, optimization of the magnet synthesis procedure involved increasing the alloy content to 20–30 wt% and adding a 20-minute isothermal step at 590 °C during SPS consolidation. Improved Tb diffusion along the grain boundaries and coercivity favorable Tb-rich core-shell microstructure led to full densification and coercivity values above 1600 kA/m in the final magnets. Conversely, using the rare-earth-lean $Nd_{33}Cu_{67}$ alloy, selected to minimize the rare-earth content in bulk magnets, lead to deteriorated magnetic performance, with coercivity value at 115 kA/m. The alloy's high melting point inhibited sufficient liquid-phase formation during sintering, leading to partial decomposition of the $RE_2Fe_{14}B$ matrix. The addition of 2.5 wt% $Nd_{70}Cu_{30}$ to $RE_2Fe_{14}B/Nd_{33}Cu_{67}$ promoted partial grain boundary wetting and microstructural stabilization, resulting in a modest coercivity increase to 160 kA/m, indicating potential for further optimization.

Acknowledgment: ARRS P2-0084, HEU REESILIENCE (101058598), GREENE (10112988).

Keywords: Nd-Fe-B magnets, Spark Plasma Sintering, Low Eutectic Alloy

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Mixed Metal Sulfates in Thermochemical Heat Storage

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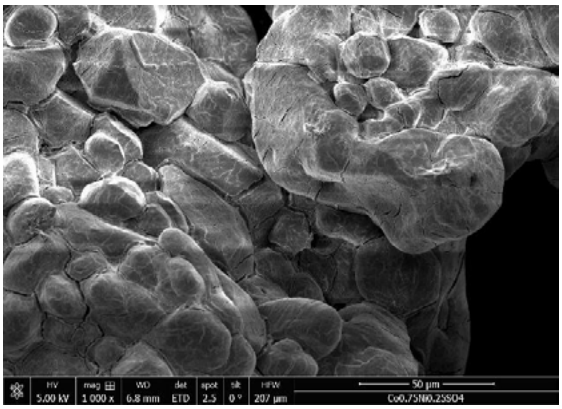
Temperatures well above 40°C in early June of this year in Spain and Portugal serve as a no longer gentle reminder that climate change poses a serious threat to the welbeing of Europe's inhabitants. In order to combat climate change despite pandemics, wars, and other crises, a wholistic approach to the energy transition is necessary. Thermochemical energy storage is an emerging technology being researched for harvesting waste heat and boasts energy storage densities higher than those of sensible heat or even latent heat storage. While many common salts such as $MgSO_4 \cdot 7H_2O$ have been investigated thoroughly, there are new discoveries to be made via chemical diversification and synthesis of new salt hydrates containing multiple different cations located in the same crystal.

One recent project involved the synthesis of a solid solution library of divalent metal sulfates of the formula $M_{1-x}M^2_xSO_4 \cdot nH_2O$ (M, M^2 = Mg, Co, Ni, Cu, Zn). Particle morphology was investigated using scanning electron microscopy. Thereby, characteristically shaped cracks were discovered some of the materials which may contribute to increased surface area and enhance reaction kinetics. Furthermore, the simultaneous thermal analysis of the synthesized salt hydrate library shed light on the dehydration behavior of various cations in this system. The high initial dehydration barrier of $NiSO_4 \cdot 6H_2O$ and the small ionic radius of nickel correpsonds to the finding that incorporation of nickel into other sulfates led to lower degrees of dehydration at low temperatures. Finally, the surprisingly facile dehydration of hydrated $Mg_{0.25}Zn_{0.75}SO_4$, is worth mentioning, as its reactivity exceeds that of both $MgSO_4 \cdot 7H_2O$ and $ZnSO_4 \cdot 7H_2O$.



Keywords: thermochemical heat storage, salt hydrates, TGA, DSC

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Kombinacija TGA–MS in komplementarnih tehnik za določitev termičnega razpada $K_2[Cu(C_2O_4)_2]\cdot 2H_2O$

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Raziskovali smo potek termičnega razpada sintetizirane koordinacijske spojine kalijevega bis(oksalato)kuprata(II) dihidrata, $K_2[Cu(C_2O_4)_2]\cdot 2H_2O$.

Na osnovi termogravimetrične analize (TGA) v atmosferi argona, smo določili stopnje razpada koordinacijske spojine in temperature, pri katerih smo pod enakimi pogoji termične obdelave pridobili štiri intermediate: 110 °C, 285 °C, 400 °C in 1000 °C, ki smo jih nadalje analizirali s TGA komplementarnimi tehnikami, rentgensko praškovno difrakcijo (XRD) in Fourierjevo transformacijsko infrardečo spektrometrijo (FT-IR). Potek razpada smo nadalje skušali določiti na osnovi analize sproščenih plinov med TGA meritvijo v atmosferi argona s sklopitvijo termogravimetrične analize z masno spektroskopijo (TGA–MS) do 1300 °C.

Na podlagi XRD in FT-IR meritev smo potrdili strukturo sintetizirane koordinacijske spojine ter določili vsebnost trdnih spojin intermediatov posameznih stopenj termične razgradnje. S TGA–MS smo potrdili razvoj enostavnih plinskih molekul H_2O, CO in CO_2, tehnika TGA pa nam je po opravljenih analizah skupaj z vsemi drugimi tehnikami omogočala predpostavko stehiometrije reakcij in intermediatov v vsaki stopnji razpada.

Ugotovili smo, da v prvi stopnji poteče popolna dehidracija, v sledečih pa razpad strukture koordinacijske spojine na kalijev oksalat, kalijev karbonat ter razne okside (CuO, Cu_2O in K_2O). Kot končni produkt termične razgradnje koordinacijske spojine pri 1300 °C pa glede na izgled preostanka in izgubo mase predpostavimo rdeč Cu_2O. Zadnjo, pri 1300 °C nedokončano stopnjo izgube mase, pripisujemo (nepopolni) sublimaciji taline K_2O, kar smo dokazali s potekom termičnega razpada spojine $K_2C_2O_4\cdot H_2O$ pri enakih pogojih merjenja.

Tekom analize rezultatov meritev komplementarnih tehnik (XRD, FT-IR) smo naleteli še na problem rehidracije preostankov po termični analizi kot tudi na MS detekcijo nepričakovanih plinskih molekul (H_2) kot posledica ravnotežnih reakcij v atmosferi TGA peči, ki so pogojeni s pogoji v celici TGA (povišana temperatura, CuO preostanek, Al_2O_3 lonček ter Pt kot del termočlena).

Ključne besede: $K_2[Cu(C_2O_4)_2]\cdot 2H_2O$, TGA, TGA–MS, XRD, FT-IR

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Diastereo-specific through-space scalar $^{19}F–^{19}F$ NMR coupling

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^{19}F NMR is a powerful technique for studying the structure, conformation, and intermolecular interactions of fluorinated compounds relevant to medicinal chemistry, materials science, and beyond.[1] Here, we report an intriguing ^{19}F NMR pattern observed in a molecule with three chiral centers bearing two CF_3 groups at tertiary and quaternary carbons. During the addition of the Rupert–Prakash reagent to the phthalimide-protected phenylalanine-derived aldehyde, a selective mono-alkylation can be achieved at −78 °C, whereas double alkylation occurs at higher temperatures.[2] The double-alkylated product was prepared on a gram scale with a diastereomeric ratio of 44:39:7:10. One of the diastereomers displayed a pentet and a quartet in the ^{19}F NMR spectrum, corresponding to the tertiary and quaternary carbon-bound CF_3 group, and the remaining diastereomers showed the expected doublet and singlet pattern. The observed ^{19}F NMR pattern can be attributed to through-space scalar $^{19}F–^{19}F$ *J*-coupling (J_{FF}). While through space J_{FF} has been documented in the literature,[3] the reports of intramolecular stereospecific long-range J_{FF} are scarce. The diastereomers were readily separated by flash chromatography on silica. Further structural elucidation by single-crystal X-ray diffraction analysis confirmed the (*R**,*R**,*S**) relative configuration with the CF_3 groups in close proximity stabilized by intramolecular H-bond. Solvent-dependent ^{19}F NMR experiments demonstrated that disruption of this hydrogen bond (in DMSO-d_6/D_2O mixtures) results in the disappearance of the scalar coupling pattern, confirming the dynamic and solvent-sensitive nature of the system. This solvent-induced conformational behavior may offer opportunities for the development of molecular sensors or switching devices based on intramolecular interaction monitoring via ^{19}F NMR. Finally, this study contributes to a deeper understanding of ^{19}F NMR and highlights its remarkable sensitivity to subtle stereochemical environments.

Keywords: ^{19}F NMR spectroscopy, Through-space scalar coupling, CF_3 groups, Diastereomers, Stereochemistry

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Stereoselektivna sinteza fluoriranih cikličnih sulfamidatov

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V zadnjih desetletjih je sinteza fluoriranih organskih spojin doživela izjemen razcvet, vendar asimetrična sinteza kiralnih fluoriranih molekul z več kiralnimi centri ostaja velik izziv.[1] Ena najobetavnejših metod za stereoselektivno pripravo takšnih spojin je asimetrično transfer hidrogeniranje (ATH), sklopljeno z dinamično kinetično resolucijo (DKR), z uporabo rutenijevih(II) ali rodijevih(III) Noyori-Ikariya katalizatorjev.

Z uporabo topnih Noyori-Ikariya katalizatorjev, mravljinčne kisline kot vira vodika in šibke organske baze kot promotorja epimerizacije smo razvili učinkovito metodo za pripravo enantiomerno čistih CF_3-substituiranih cikličnih sulfamidatov. Izhodiščne racemne 4-substituirane 5-(trifluorometil)-5*H*-1,2,3-oksatiazole smo sintetizirali iz α-hidroksi-trifluorometil ketonov prek reakcije s sulfamoil kloridom. Ti intermediati so dostopni bodisi s kaskadnim aciliranjem, premestitvijo in dekarboksilacijo α-hidroksi karboksilnih kislin z anhidridom trifluoroocetne kisline[2] bodisi z NHC-katalizirano benzoinsko kondenzacijo.[3]

Reakcijske pogoje smo najprej optimizirali na modelnem 4-fenil substituiranem oksatiazolu, nato pa razširili nabor substratov na različno substituirane aromatske in heteroaromatske spojine ter zahtevnejše alifatske derivate. Močna elektronska privlačnost skupine CF_3 je omogočila učinkovito epimerizacijo že z uporabo šibke baze, kar je bistveno olajšalo DKR proces.

Enantiomerno čistost produktov smo določali s kiralno HPLC ali GC analizo. Za aromatske derivate smo dosegli izjemno visoke vrednosti ee (nad 99 %), medtem ko so bili rezultati za alifatske substituente prav tako zelo dobri (nad 95 % ee). Slednje kaže na mehanizem kontrole stereoselektivnosti, ki odstopa od kanonične CH–π interakcije, značilne za to vrsto katalize.[4]

Predstavljena metoda ponuja robustno platformo za pripravo kompleksnih, kiralnih fluoriranih gradnikov, ki so potencialno uporabni v razvoju bioaktivnih molekul in farmacevtskih učinkovin.

Ključne besede: asimetrično transfer hidrogeniranje, dinamična kinetična resolucija, fluor, rodij, razvoj učinkovin

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Phospholipid Profiling: A Computationally Assisted LC-HRMS Approach

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Phospholipids are amphiphilic molecules consisting of various polar head groups and non-polar fatty acid tails that differ in chain length and saturation. As basic components of cell membranes, they self-assemble into bilayers in all living organisms. Due to their structural versatility, phospholipids are often used as natural emulsifiers and encapsulating agents in pharmaceutical, food and cosmetic applications. In these formulations, they promote the formation of micelles and liposomes and thus improve the stability, bioavailability and delivery of active ingredients [1].

Lecithin, a common industrial source of phospholipids, has functional properties that are highly dependent on its phospholipid composition. Variations in head groups and fatty acid saturation influence the ability of lecithin to form specific structures and determine its emulsifying behavior. Accurate profiling of phospholipid content is therefore critical to product performance and stability [2].

Conventional analysis relies heavily on commercial reference standards. However, the structural diversity of phospholipids requires a wide range of standards, which are often costly, scarce and time consuming to use effectively in complex samples such as lecithin [3].

In this study, a qualitative, standard-free method for the identification of phospholipids in lecithin is presented. Reversed-phase high-performance liquid chromatography was coupled with high-resolution mass spectrometry to separate and detect the phospholipid species. Molecular ions were recorded in full-scan mode and analyzed using a custom Python script that generated a list of possible phospholipid structures for each m/z value. The identification was confirmed by matching the MS/MS fragmentation patterns with the theoretical predictions.

The proposed workflow provides a reliable and cost-effective alternative for phospholipid profiling in complex lipid matrices and demonstrates the feasibility of standard-free identification using advanced analytical and computational tools.

Keywords: phospholipids, lecithin, HPLC, LC-HRMS

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Discovery of Potent Novel Bacterial Topoisomerase Inhibitors with Reduced hERG Toxicity

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Life-threatening hospital bacterial infections are caused by escalating resistance to Gram-positive and Gram-negative pathogens which resulted in many emerging classes of antibacterial compounds against well-validated bacterial targets, such as DNA gyrase and topoisomerase IV [1,2]. Novel bacterial topoisomerase inhibitors (NBTIs) consist of the left-hand-side (LHS) moiety which intercalates in DNA, the linker that ensures a correct spatial orientation and appropriate physicochemical properties of the ligand, and the right-hand-side (RHS) moiety, which interacts with the GyrA subunits of the enzymes. NBTIs suffer from the class-related hERG blockage tendency, which is clinically manifested as ventricular tachyarrhythmia and prevents more potent NBTIs from progressing to clinical trials. Consequently, the reduction of hERG inhibitory activity by tuning of NBTI's physicochemical properties is necessary to develop potential clinical candidates. NBTIs tend to be less potent against Gram-negative bacteria, such as *Escherichia coli*, due to their relatively high substrate specificity for the bacterial efflux pumps, which is another potential direction of development of NBTI chemotypes [2,3].

We aim to develop DNA gyrase inhibitors with high on-target potency and antibacterial activity against Gram-negative bacteria with an acceptable hERG inhibitory profile. We selected some of the most progressive NBTIs from the literature and conducted serial substitution of their RHS moieties with RHSs proposed by a machine-learning-based model DeepFrag. The generated RHS moieties were converted to aldehydes and carboxylic acids and filtered to resemble physicochemical properties of known RHS moieties from potent and toxicologically safe NBTIs. Virtual combinatorial reactions between aldehydes and carboxylic acids and known NBTI scaffolds were enumerated and the products were filtered with drug-likeness filters (Lipinski/Veber rule sets). Their inhibitory activities on hERG were predicted utilising Pred-hERG. Molecular docking calculations of the selected NBTIs with acceptable hERG profiles were conducted by using the available DNA gyrase structural data originating from *E. coli* and *Staphylococcus aureus*. All systems were further subjected to molecular dynamics simulations and their free energies of binding were predicted by the linear interaction energy method. This drug discovery workflow resulted in novel NBTI chemotypes with predicted nanomolar inhibitory potencies on *E. coli* and *S. aureus* DNA gyrase with an acceptable potency/hERG toxicity ratio.

Keywords: novel bacterial topoisomerase inhibitors; Gram-negative bacteria, hERG inhibition

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Novel bacterial topoisomerase inhibitors with reduced toxicity and improved *in vitro* and *in vivo* efficacy

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Bacterial type II topoisomerases are crucial bacterial enzymes and have long been validated as targets for antibacterial therapy. Although fluoroquinolones are the most widely used inhibitors of these enzymes, their clinical effectiveness is steadily declining due to the increasing prevalence of resistance. In contrast, novel bacterial topoisomerase inhibitors (NBTIs) represent a structurally diverse class of compounds that bind to a different site and act through a distinct mechanism, thereby avoiding cross-resistance with quinolones [1]. Recently, gepotidacin was the first NBTI to be approved by the FDA. Unfortunately, the development of most other NBTIs is often halted early due to their tendency to inhibit hERG potassium channels, which can lead to potentially fatal cardiac arrhythmias [2,3]. To address this challenge, we carried out structural and physicochemical modifications of the DNA-intercalating region of NBTIs to enhance antibacterial potency while reducing cardiotoxic risk. The resulting compounds were tested for minimum inhibitory concentrations (MICs) against a panel of Gram-positive and Gram-negative bacteria. Several of the compounds from our new series, demonstrated lower MICs compared to gepotidacin and also showed strong inhibitory activity against topoisomerase IV and DNA gyrase from both *Escherichia coli* and *Staphylococcus aureus*. Some of our best compounds were also tested in the fish embryo acute toxicity test, and exhibited no or only sublethal toxicity. Additionally, in a zebrafish infection model with *S. aureus*, the tested compound successfully eradicated the infection at sub-toxic doses, highlighting its potential as a promising lead for further antibacterial drug development.

Keywords: antibiotics, antibacterials, topoisomerase type II inhibitors, NBTIs, bacterial drug resistance

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Protonation Dynamics of a Doubly Reduced Biomimetic FeFe-Hydrogenase Catalyst

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The transition to a carbon-free society necessitates efficient catalysts for hydrogen (H_2) production. Biomimetic FeFe-hydrogenase catalysts, inspired by nature's highly active enzymes, are promising candidates. This study investigates the protonation dynamics of the doubly reduced species ($\mathbf{1}^{2-}$) of the biomimetic catalyst $Fe_2(\mu\text{-ADT})(CO)_6$ (**1**), a key intermediate in H_2 evolution under strongly reducing conditions. Using stopped-flow Fourier transform infrared (FTIR) spectroscopy, we characterized the metal-protonated doubly reduced species, identified by an ~80 cm^{-1} absorption band shift, after reacting $\mathbf{1}^{2-}$ with phenol and 4-(trifluoromethyl)-phenol. With a large excess of 4-(trifluoromethyl)-phenol or a strong acid (pentachlorophenol), a second protonation event occurred, leading to H_2 evolution and catalyst turnover. This sets the pKa threshold for catalytic turnover at around 25. Upon reductant depletion, only the first reduction was reached, producing $\mathbf{1}^{-}$, which immediately disproportionated, dimerized, and formed degradation products in the presence of a proton source. Understanding the proton reduction mechanism provides valuable insights for future research into optimizing the catalyst design to influence the reactivity, basicity, and stability of the key intermediates.

Keywords: Biomimetic hydrogenase catalyst, time-resolved FTIR, stopped-flow, doubly reduced complex

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From Inert to Bioactive: Natural Compound-Based Modification of Bacterial Nanocellulose for Burn Wound Care

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Bacterial nanocellulose (BnC) – a biopolymer synthesised as an extracellular polysaccharide by various non-pathogenic bacteria, garnered significant interest in burn wound care due to its exceptional properties, including ultra-high purity, high water-holding capacity, excellent biocompatibility, non-toxicity and mechanical stability [1]. However, a significant limitation of native BnC is its lack of bioactivity, a challenge that may be addressed through the incorporation of bioactive compounds into the BnC matrix. While prior studies have examined the application of BnC as a burn wound dressing, the investigation of real-time interactions using quartz crystal microbalance with dissipation monitoring (QCM-D) and the assessment of BnC's toxicity in combination with natural bioactive compounds within ex vivo human skin explants remains an unexplored field of material science [2].

This study focused on modifying BnC in situ by carboxymethyl cellulose to introduce a carboxyl group to the BnC matrix and therefore facilitate further ex-situ modification using natural bioactive compounds – bromelain and nisin – to enhance the membranes with proteolytic and antimicrobial properties. BnC-CMC nanocrystals were synthesised from BnC-CMC membranes and were subsequently utilised to investigate surface interactions with bromelain and nisin using QCM-D methodology. The membranes were comprehensively evaluated according to physical-chemical, morphological, mechanical, and both in vitro and ex vivo bioactive properties to determine any cellular damage and skin irritation caused by topical application on human skin explants, providing an ethical approach for studying burn wound healing.

Keywords: bacterial nanocellulose, bioactive, burn wound care, nisin, bromelain

Acknowledgement: The authors would like to thank the Slovenian Research and Innovation Agency for funding this research through the Young Researcher Program (P2-0118/0795), project N2-0388 and Horizon EU project NABIHEAL (n°101092269). The authors are grateful to Prof. dr. Janja Trček for providing the bacterial strain through the Microbial Culture Repository of the Faculty of Natural Sciences and Mathematics, University of Maribor.

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Biokompatibilni materiali v ekstremnih dentalnih pogojih: primer cirkonija ob prisotnosti HCl

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Zobni implantati, kot ključna rešitev v sodobni zobozdravstveni protetiki, morajo združevati mehansko trdnost, korozijsko odpornost in biokompatibilnost, saj so stalno izpostavljeni zahtevnim razmeram v ustni votlini. Cirkonij in njegove zlitine se uveljavljajo kot obetavna alternativa tradicionalnim materialom, saj tvorijo stabilno zaščitno oksidno plast (ZrO_2), ki omogoča visoko korozijsko odpornost, tudi v prisotnosti agresivnih snovi. Veliko novejših študij je opravljenih na zlitinah, ki ob cirkoniju vsebujejo tudi titan, ki je največkrat uporabljen biokompatibilni element.

Za dolgoročno stabilnost vsadkov je ključna odpornost materiala na agresivne razmere v ustni votlini – med drugim tudi na morebitno prisotnost želodčne kisline, ki vanjo zaide pri bolnikih z gastroezofagealnim refluksom. Želodčna kislina (HCl) je močna anorganska kislina, ki lahko ob dolgotrajni izpostavitvi povzroča poškodbe – korozijo tudi najbolj odpornih materialov.

Zaradi tvorbe stabilne zaščitne plasti cirkonijevega oksida (ZrO_2) kaže cirkonij obetavne rezultate tudi v teh ekstremnih pogojih. Njegovo obnašanje v prisotnosti želodčne kisline je zato ključnega pomena za oceno njegove varnosti in učinkovitosti kot dolgoročne rešitve v zobozdravstveni protetiki.

Za oceno korozijske odpornosti cirkonija smo pripravili poskus, v katerem so bili vzorci pri telesni temperaturi (37 °C) izpostavljeni umetni slini, z dodano klorovodikovo kislino (HCl) v koncentracijah 0,1, 0,01, 0,001 in 0,0001 mol/L, ki ustrezajo pH vrednostim 1, 2, 3 in 4, s čimer smo simulirali pogoje, ki lahko nastopijo pri gastroezofagealnem refluksu. Spremembo mase vzorcev pred in po izpostavitvi smo kvantitativno ovrednotili z gravimetrično metodo ter izračunali hitrost korozije po 24, 48, 72 in 96 urah. Za vizualizacijo morfoloških sprememb na površini materiala smo uporabili vrstični elektronski mikroskop (SEM), kar je omogočilo vpogled v naravo in obseg površinske degradacije.

Ključne besede: Cirkonij, umetna slina, dentalni implantati, želodčna kislina

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Proton exchange membranes based on bacterial cellulose and graphene oxide for microbial fuel cells

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Microbial fuel cells (MFC) [1] are a promising bioelectrochemical technology for simultaneous wastewater treatment and electricity generation. However, the widespread application of MFCs is hampered by limitations in membrane performance, particularly in terms of proton conductivity, mechanical integrity and resistance to biofouling. Bacterial cellulose (BC), a natural biopolymer mainly produced by *Acetobacter species* [2], exhibits high mechanical strength and excellent water-holding capacity, making it a suitable candidate for membrane separators in MFCs. Nevertheless, its low proton conductivity and susceptibility to biofouling require further modification. To address these limitations, graphene oxide (GO) [3], known for its high surface area, oxygen-containing functional groups and antibacterial properties, was incorporated into the BC matrix to produce BC-GO composite membranes. The membranes were prepared by mixing BC and GO dispersions with different GO concentrations (0–0.075 wt%) followed by casting and drying. A comprehensive characterisation was carried out with regard to morphology (Figure 1), crystallinity, chemical composition, thermal and mechanical stability, swelling behaviour, ion exchange capacity (IEC) and ionic conductivity. It was found that the addition of GO maintains the BC nanofibrilar structure, increases the thermal stability and Tensile strength and improves the IEC. These results demonstrate the potential of bio-based BC-GO membranes as sustainable and efficient separators for next-generation MFC technologies.

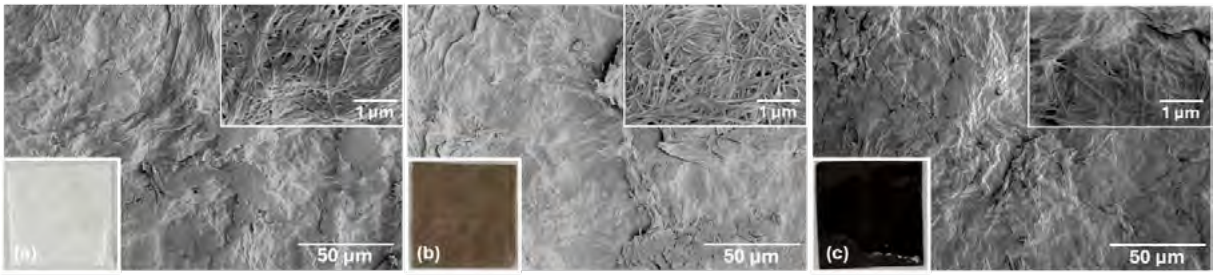

Figure 1: Digital (figure inserts) and different magnification FE-SEM images of BC membranes without (a) and with 0.01 wt%, (b) and 0.05 wt% (c) GO concentration.

Acknowledgment: The authors would like to acknowledge the financial support from Slovenian Research and Innovation Agency (ARIS), in frame of projects J2-50086, Z2-60175 and Young researcher program in frame of Textile Chemistry and Advanced Textile Materials Programme (P2-0118).

Keywords: bacterial cellulose, fuel cell, proton exchange membrane, graphene oxide

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Reactive Sorbents for Ammonia Synthesis: Performance of Magnesium Chloride-Based Materials

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Ammonia is gaining attention as a promising carbon-free energy carrier due to its high energy density and compatibility with existing infrastructure. However, conventional ammonia synthesis is energy-intensive and incompatible with the intermittent nature of renewable energy [1]. In particular, the separation of ammonia by condensation requires a considerable amount of energy. Sorbent-enhanced ammonia synthesis offers a potential solution by integrating reactive separation using solid sorbents, thus enabling more energy-efficient operation. Among various materials, metal halides have shown high ammonia uptake and good reversibility through coordinative absorption [2,3]. Nevertheless, their practical application is hindered by the structural degradation caused by up to 400% volume expansion during absorption, leading to sintering and agglomeration, especially at elevated temperatures. To overcome these challenges, metal halides are often dispersed on porous supports with large surface area to improve thermal stability and maintain sorption performance [4].

This study investigates $MgCl_2$-impregnated porous materials as advanced sorbents for ammonia capture, focusing on efficient material characterisation under inert conditions and the development of a novel kinetic model for ammonia absorption and desorption. Various porous supports were impregnated with $MgCl_2$ *via* the wet impregnation method and their performance was evaluated by breakthrough experiments. Of the materials tested, $MgCl_2$/ZSM-5 and $MgCl_2$/USY (Si/Al = 500) showed the highest ammonia uptake at 25 °C, although the sorption capacity decreased with increasing temperature. These sorbents showed stable performance over 10 absorption/desorption cycles, emphasising their potential for sorbent-enhanced ammonia synthesis. The results show that the ammonia sorption capacity strongly correlates with the pore size distribution. Supported $MgCl_2$ sorbents retain their structural integrity and show improved kinetics. These results demonstrate the potential of $MgCl_2$-supported materials for efficient, regenerable ammonia separation in industrial settings. Improved high-temperature performance and careful tuning of support chemistry, particularly porosity and acidity, are key to improving sorption capacity and stability for ammonia storage and sorption applications.

Keywords: ammonia separation; sustainable energy; metal halides; kinetic modeling

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Catalytic Conversion of CO_2 to Propylene Carbonate over Hydrotalcites-derived mixed metal oxides

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One promising approach for CO_2 utilization in organic transformations is the synthesis of propylene carbonate via a tandem epoxidation/cycloaddition reaction [1]. This process is considered a highly attractive industrial process due to its atom economy, cost-effectiveness, and inherent safety. However, this transformation must be carried out in the presence of an efficient catalyst, due to the low reactivity of CO_2 [2]. In this study, a series of Zn-Mg-Al mixed oxides derived from layered double hydroxides have been synthesized and evaluated as a catalyst for the synthesis of propylene carbonate (PC) from CO_2 and propylene oxide. The Zn/Mg molar ratio significantly influences the physiochemical properties of the catalysts such as crystallite size, surface area, and CO_2 adsorption capacity. Under optimized conditions, the catalyst with a Zn/Mg molar ratio of 3 exhibits the highest conversion (96.8%) of propylene oxide and propylene carbonate selectivity (82.4%). The catalyst also maintained consistent performance over three cycles, highlighting its potential as a stable, reusable, and environmentally friendly catalytic system for CO_2 cycloaddition.

Keywords: Propylene carbonate, CO_2 Cycloaddition, Layered double hydroxides, Epoxidation, and mixed oxides.

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Catalytic Performance of Supported Metal Oxides in Dielectric Barrier Discharge Plasma for Ammonia Production

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Ammonia is widely used in fertilizer production, but is also gaining attention as a potential energy carrier in various sectors. However, this transition requires a sustainable alternative to the centralized, energy-intensive Haber-Bosch. Plasma-catalytic systems offer a promising solution as they are compatible with intermittent renewable energy and are suitable for on-site small-scale production. Despite their potential, these systems are still limited by the low energy efficiency.[1] In recent years, research has mainly focused on metal catalysts supported by porous materials. Micro- and mesoporous materials enhance diffusion of the plasma-activated species to the active sites. Additionally, the use of porous supports has been shown to improve overall efficiency of ammonia production due to the "shielding effect", where produced ammonia is protected from plasma-induced decomposition by diffusion inside the pores.[2] Catalysts with Co, Ni and Ru are most commonly utilized as these metals have shown the best catalytic performances in DBD plasma-catalytic systems. However, the synthesis of such materials requires an additional reduction step, which can lead to an increase in the size of the metal particles, reducing the activity of the catalyst. In addition, transition metal nanoparticles are often prone to partial oxidation in air due to their high surface energy [3]. In this study, supported metal oxides are investigated as alternative catalysts for DBD plasma-catalytic ammonia production using USY zeolite as a support with well-defined pore structure, high surface area and stability. To systematically evaluate the effects of the synthesis method on the catalytic performance, the best performing catalyst was synthesized using both wetness impregnation and precipitation method. The characterization revealed that precipitation method produces smaller metal oxide particles, which correlated with higher catalytic activity. Among the tested materials, cobalt and nickel oxides demonstrated the best performance, which is consistent with previously observed activity trends for transition metal catalysts.

Ključne besede: ammonia, metal oxides, nitrogen fixation, plasma-catalysis

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CFD Analysis of Internal Diffusion Effects in a Single Catalytic Pellet

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Proper modelling of heterogeneous catalytic reaction and reactor design optimization depends heavily on a realistic representation of the internal mass transfer phenomenon [1]. This study employs computational fluid dynamics (CFD) to investigate diffusion limitations in CO oxidation in a single catalytic particle with two modelling schemes: The Instantaneous Diffusion Model (IDM), which assumes reactions occur only on the outer surface with no resistance within the interior, and the Porous Media Model (PMM), which includes coupled diffusion and reaction through the catalyst volume [2]. The reaction system is CO oxidation on Rh/Al_2O_3 modelled by a five-step reversible mechanism [3]. The experiments were conducted under isothermal, laminar flow conditions in a tubular reactor containing a centrally positioned catalyst pellet. The PMM allowed spatial resolution of concentration and reaction gradients within the porous regime, which was seen to exhibit strong internal mass transfer limitations under conditions of high surface reactivity and high volume-specific surface area (VSSA). To enhance the predictive power of the IDM at the cost of little computation, effectiveness factors were obtained from PMM simulations and used to adjust the surface area for reaction in the IDM by a corrected washcoat factor. This adjustment enabled the reduced model to capture PMM conversion trends at the expense of computational time being decreased up to 50%. The results confirm that intrinsic diffusion limits substantially suppress reaction rates under certain circumstances and must be accounted for in low-order models to give a realistic performance projection. The factor by which the effectiveness factor was highly sensitive to catalyst characteristics, going towards zero in regimes of diffusion limitation. The improved IDM technique offers a computationally efficient and stable solution for initial-stage catalyst screening and for rigorous reactor model simulations where high-resolution PMM may be impractical. The methodology demonstrated is advantageous to the quick evaluation of catalytic systems and aids in obtaining improved process design through more effective and precise simulation of internal transport phenomena.

Keywords: CFD, Porous catalyst modelling, Effectiveness factor, Internal mass transfer, Catalytic CO oxidation

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Termokemijska valorizacija lanene pogače s hidrotermično pretvorbo

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Zaradi vse večjih potreb po trajnostnih virih energije in zmanjševanju emisij toplogrednih plinov postaja iskanje alternativ fosilnim gorivom vse pomembnejše. Biomasa predstavlja, zaradi svoje obnovljivosti, dostopnosti in možnosti za učinkovito energetsko izrabo, eno najpomembnejših alternativ za zamenjavo fosilnih goriv.[1] V zadnjih letih se povečuje zanimanje za lignocelulozne vire, kot so oljne pogače, ki nastajajo pri proizvodnji rastlinskih olj. Lanena pogača, ki je stranski produkt v proizvodnji lanenega olja, je bogata s hranili, vlakninami, maščobami in beljakovinami ter pogosto ostane neizkoriščena, saj se uporablja predvsem kot krmilo ali konča med odpadki, kar predstavlja okoljsko breme. Zaradi lignocelulozne sestave pa lahko nudi tudi pomemben potencial za nadaljnjo predelavo v različne energetsko in kemijsko zanimive produkte. Ena izmed okoljsko in tehnološko učinkovitih metod pretvorbe takšnih ostankov je uporaba pod- in nadkritične vode, s pomočjo katere lahko iz lanene pogače pridobimo bio-olja, bio-plin in bio-oglje [2].

Razgradnjo lanene pogače s pod- in nadkritično vodo smo izvajali pri treh različnih temperaturah (300 °C, 350 ° in 400 °C) in štirih različnih časih (30 min, 60 min, 90 min in 120 min). Kot produkt smo dobili trdno, oljno, vodno in plinsko fazo, med katerimi je v vseh eksperimentih prevladovala oljna faza. Najvišji izkoristek oljne faze smo dosegli pri najmilejših pogojih (300 °C in 30 min) in je znašal kar 72,3 %. Z nadaljnjim podaljševanjem časa in višanjem temperature pa je izkoristek oljne faze pričel upadati in je dosegel najnižjo vrednost pri 400 °C in 120 min (50 %). Prav tako sta upadala tudi izkoristka trdne (10 % - 3 %) in vodne faze (13 % - 4%), medtem ko je izkoristek plinske faze, kot pričakovano, s temperaturo in časom naraščal in je pri 120 min in 400 °C dosegel najvišjo vrednost (42,5 %). S pomočjo GC/MS metode smo določili kemijsko sestavo plinske in oljne faze. Plinske mešanice so po večini vsebovale CO_2 in ogljikovodike C_1-C_6. V oljnih fazah pa smo določili prisotnost alkanov, alkenov, aromatov, ketonov, estrov, kislin, amidov in ostalih dušikovih komponent, med katerimi je pri 300 °C nastalo največ amidov, med tem ko se je koncentracija aromatov in ketonov povečevala z višanjem temperature. Oljnim fazam smo določili tudi zgornje kurilne vrednosti, katere so se gibale v območju od 24 do 32 MJ/kg. S TOC analizatorjem smo v vodnih fazah določili koncentracijo skupnega ogljika in s HPLC analizo še prisotnost furfuralov. Iz FTIR spektrov trdnega produkta smo opazili, da so s hidrotermično razgradnjo razpadle glavne O-H, C=O, C-N in C=C vezi, ki so bile prisotne v neobdelani laneni pogači. Ohranile so se le nekatere vezi (C-H in C-O), ki pa so z višjo temperaturo postajale manj intenzivne. Pridobljeni podatki temeljite analize sekundarnih produktov, ki so nastali pri hidrotermični razgradnji lanene pogače v pod- in nadkritični vodi, predstavljajo pomemben korak k razvoju učinkovitih alternativnih biogoriv.

Ključne besede: lignocelulozna biomasa, lanena pogača, pod- in nadkritična voda, kemijska pretvorba, biogoriva.

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Reactivity of α-pinene oxide with acetic anhydride for one-pot synthesis of carvyl acetate

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α-Pinene oxide is very interesting compound. It may be used for synthesis of wide spectrum of substances with a variety of applications. Final products had significant utilization, e.g., in perfumery and pharmaceutical industry. When α-pinene oxide as representant of monoterpene oxides reacts with acetic anhydride, many products are formed. This reaction must be catalysed, usually by acid catalyst and proceeds in two steps as one-pot: first isomerization, and second acetylation of formed monoterpenic alcohols. When suitable conditions are applied, final acetates are produced with high selectivity. This way of preparation of monoterpenic acetate was slightly studied. Štekrová et al. [1] used β-pinene oxide under a catalysis by montmorillonite K10, the main product was perrilyl acetate with a small amount of myrtenyl acetate. Tatarova et al. [2] investigated the reactivity of α-pinene oxide, acetates were obtained at small amounts, no additional solvent were not used. Some works describing isomerization of α-pinene oxide mentioned the positive effect of basic solvent on the direct production of monoterpenic alcohols [3]. In this work, we want to show the selective preparation of carvyl acetate, which is used as sweet minty aroma and in dental hygiene [4], from α-pinene oxide. For this study, we have chosen zeolite H-Beta 25 as heterogeneous catalyst. We investigated several parameters to optimize the reaction conditions: amount of catalyst, type and amount of solvent, ratio of reactants, and temperature. We also performed scale-up and repeatability studies. Based on our findings about isomerization of monoterpenic oxide and acetylation of alcohols,we obtained the best yield of carvyl acetate (47 %) at conditions: 20 wt% zeolite H-Beta 25, ratio α-pinene oxide:acetic anhydride:*N*,*N*-dimethylformamide = 1:8:8, 90 °C, 4 h. The main by-product was campholenic aldehyde (25 % yield), which is a significant reactant for synthesis of compounds with santal wood fragrance. We also evaluated kinetics (reaction rate constants and activation energies).This work contributes to better understanding of a reaction between α-pinene oxide and acetic anhydride generally, but also provides new way of synthesis of carvyl acetate.

Keywords: one-pot synthesis; α-pinene oxide; carvyl acetate; heterogeneous catalysis; acid catalysis

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Immobilization of Invertase on Porous Poly(HEMA-co-MBAA) Monoliths for Efficient Hydrolysis of Sucrose

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Poly(2-hydroxyethyl methacrylate) (polyHEMA)-based materials have attracted considerable interest due to their biocompatibility, hydrophilicity, and tunable physicochemical properties. Their hydroxyl-functionalized backbone enables chemical modification, allowing the introduction of functional groups for biomedical and biotechnological applications. In biomedical engineering, polyHEMA hydrogels are commonly used as scaffolds in tissue engineering, contact lenses, and drug delivery systems, primarily because of their high-water content, mechanical flexibility, and non-toxicity. Copolymerization or surface modification can further enhance these materials by improving mechanical strength, cell adhesion, or bioactive functionality. [1]

Enzyme immobilization on polyHEMA-based materials can be achieved via covalent attachment (directly or after activation with agents such as glutaraldehyde), non-covalent interactions (e.g., hydrogen bonding, electrostatic attraction, van der Waals forces), physical entrapment, encapsulation, or cross-linking of enzyme aggregates. These methods improve enzymatic stability, activity, and reusability. In many immobilization strategies, the porosity of the material is a crucial factor as it facilitates the effective entrapment and stabilization of the enzymes within the internal structure. [2]

A highly effective method for generating porosity in polymeric materials is high internal phase emulsion (HIPE) polymerization. This technique involves emulsifying two immiscible liquids, with the internal phase typically exceeding 74% of the total volume. Polymerization of the continuous phase yields a macroporous polyHIPE structure with large, interconnected pores originating from the dispersed droplets. This architecture is well suited for enzyme immobilization due to its high surface area and accessible porous network. [3]

In this work, a porous poly(HEMA-co-MBAA) monolith was synthesized via HIPE polymerization, using an emulsion composed of 80 vol% internal phase and 15 mol% *N,N'*-methylenebisacrylamide (MBAA) as the crosslinking agent. The resulting material was employed for invertase immobilization, and its catalytic performance in the hydrolysis of sucrose was evaluated. Kinetic parameters were determined, and the effects of pH and temperature on enzyme activity were investigated.

Keywords: porous polymers, polyHIPEs, immobilised enzymes, invertase, hydrolysis

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Zeolit kot nosilec za imobilizacijo encima invertaza

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Biokatalizatorji, med katere spadajo encimi, omogočajo specifične kemijske pretvorbe pri blagih reakcijskih pogojih, so okolju prijazni ter energetsko učinkoviti. V industriji so posebej uporabni imobilizirani encimi, saj imobilizacija omogoča lažje ločevanje encima iz reakcijske zmesi, izboljšano stabilnost (termično, mehansko, kemično) in večkratno uporabo biokatalizatorja.[1]

Pri našem delu smo se osredotočili na imobilizacijo encima invertaze. Invertaza (β-fruktofuranozidaza) katalizira hidrolizo saharoze v glukozo in fruktozo, kar imenujemo invertni sirup. Ta reakcija je pomembna v živilski industriji pri proizvodnji sladil, sirupov in farmacevtskih izdelkov.[2] Encim invertazo smo imobilizirali na zeolit (proizveden v Silkem). Zeoliti so mikroporozni aluminosilikatni minerali z visoko specifično površino, ionsko izmenjevalno kapaciteto in stabilno strukturo, kar omogoča učinkovito vezavo encimov.[3]

Zeolitni nosilec z imobiliziranim encimom smo okarakterizirali z različnimi metodami. S SEM smo preverili morfologijo in porazdelitev delcev zeolita, s FTIR spektroskopijo smo potrdili prisotnost značilnih funkcionalnih skupin, z elementno analizo smo določili vsebnost nekaterih kemijskih elementov. Analizo vzorcev reakcijskega medija smo izvajali s HPLC. Spremljali smo koncentracentracijske profile saharoze, glukoze in fruktoze v različnih časovnih intervalih. Preverili smo vpliv pH reakcijskega medija in temperature na presnovo saharoze.

Iz rezultatov je razvidno, da je bila imobilizacija invertaze na zeolit uspešna. Ohranili smo visoko encimsko aktivnost in učinkovitost reakcije hidrolize saharoze. Z imobiliziranim encimom smo izboljšali stabilnost in omogočili večkratno uporabo, kar potrjuje uporabnost imobilizirane invertaze pri različnih industrijskih procesih.

Ključne besede: encim, imobilizacija, invertaza, zeoliti.

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Tracing nanoplastics removal dynamics: Europium-labeled polystyrene adsorption on fungal biomass in a simulated treatment system

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Nanoplastics (NPs), defined as synthetic polymer particles of size in the submicron range, are emerging as pervasive environmental contaminants owing to their tendency to cross biological membranes and bioaccumulate within ecological systems, thereby posing considerable risks to environmental safety and human health. Their small size (< 1 μm) challenges conventional separation and analytical methods, presenting the need for innovative and sustainable detection [1]. This study presents a novel approach for the remediation of polystyrene nanoplastics (PSNPs) by employing fungal biomass as an adsorbent for their removal. Fungal materials are natural, renewable, biodegradable, and inexpensive, with diverse functional groups on cell walls that can facilitate pollutant binding [2]. The medicinal mushroom *Trametes versicolor* has been employed based on proven ability to bind various contaminants, although its role in nanoplastic removal remains underexplored. To accurately track and quantify PSNPs during adsorption experiments, europium-doped PSNPs (Eu-PSNPs) [3] were employed for a precise monitoring of PSNPs adsorption and removal mechanism based on the quantification of Eu by inductively coupled plasma-optical emission spectroscopy (ICP-OES). Initially, microwave-assisted acid digestion and ICP-OES elemental analysis was conducted to verify the absence of Eu in the fungal biomass, thereby confirming its suitability as a marker. Batch experiments we used to investigate the effect of contact time and fungal mass on the adsorption. Adsorption efficiency increased steadily with contact time, plateauing at approximately 63.1% of Eu-PSNPs removal. As expected, increasing the mass of fungal material led to a higher removal efficiency, reaching an 77.7% efficiency, attributed to a larger number of available adsorption sites. To simulate real-environmental applications, such as continuous water filtration, a column setup was employed, achieving significantly higher adsorption efficiencies than batch experiments. In this system, PSNPs levels in the effluent dropped below detectable limits, indicating near-complete (i.e. > 99%) removal. Laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) analysis confirmed that Eu-PSNPs particles were retained in the column of fungal biosorbate, demonstrating good potential for polystytene nanoplastics removal. The adsorption behaviour was further evaluated by Freundlich-Langmuir isotherm (K_L = 26.9 L mg^{-1}), reflecting both surface heterogeneity and saturation effects. The kinetics of the adsorption process were best fitted by the pseudo-first-order kinetic model (k_1 = 1.4 min^{-1}), indicating physisorption as the primary mechanism. This study demonstrates a sustainable approach for PSNPs remediation using *Trametes versicolor*, effective under dynamic conditions with binding affinity for nanoplastics. This study also presents an example of precise nanoplastics tracking strategy, based on Eu-doped PSNPs, supporting green chemistry and further environmental research on water remediation and reuse applications.

Keywords: Nanoplastics, Remediation, Fungal biosorption, *Trametes versicolor*, Water treatment

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Energetska izraba ostankov fermentacije v trdnem stanju

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Povzetek

Zaradi omejenih zalog fosilnih goriv in hkrati vse večjih potreb po energiji, se svet vse bolj usmerja v iskanje trajnostnih, obnovljivih virov. Uporaba fosilnih goriv prispeva k številnim okoljskim težavam, kot so emisije toplogrednih plinov in onesnaženje, iz ekonomskega vidika pa ima pomemben vpliv tudi politična odvisnost glede zalog nafte in plina [1]. Eden od alternativnih virov, ki izstopa po dostopnosti in količini je lignocelulozna biomasa. Ta predstavlja pomemben vir energije, a zaradi svoje specifične zgradbe oz. sestave zahteva dodatne postopke obdelave. V zadnjem času se vse bolj uveljavlja uporaba kombiniranih postopkov, ki vključujejo različne fizikalne, kemijske, termične in biološke pristope za izboljšanje predelave lignocelulozne biomase. Biološka obdelava omogoča učinkovito razgradnjo kompleksnih komponent biomase, kot so npr. lignin, celuloza in hemiceluloza, ter poveča dostopnost biomase za nadaljnjo energetsko izrabo [2,3]. K naprednejšim postopkom obdelave biomase prištevamo tudi pirolizo, termo-kemijski proces razgradnje materiala v odsotnosti kisika, pri katerem nastajajo trdni, tekoči in plinasti produkti. Ta postopek ne omogoča le energetske izrabe, temveč tudi zmanjšanje količine odpadkov in pridobivanje produktov z dodano vrednostjo [4].

V tej raziskavi smo preučevali možnosti energetske izrabe ostankov, ki nastanejo po biološki obdelavi lignocelulozne biomase. Kot izhodiščni material smo uporabili odpadek iz industrije rastlinskih olj, ki je bil predhodno biološko obdelan z glivami v procesu fermentacije v trdnem stanju *(angl. solid state fermentation - SSF*). Namen raziskave je bil ovrednotiti, kako časovna komponenta biološke obdelave vpliva na nadaljnjo termično pretvorbo biomase, natančneje na proces pirolize. Pirolizo smo izvedli pri dveh različnih temperaturah v inertni (N_2) atmosferi in analizirali nastale trdne in plinaste produkte. Učinke biološke obdelave smo ovrednotili s primerjavo rezultatov z biološko neobdelanim vzorcem. Karakterizacijo surovin in trdnih produktov smo izvedli z elementno analizo, FTIR spektroskopijo, določitvijo kurilne vrednosti ter analizami vsebnosti hlapnih snovi, vlage in pepela. Z namenom, da bi preučili termično stabilnost obdelanih vzorcev, smo vzorce dodatno izpostavili termogravimetrični analizi (TGA).

Ključne besede: energetska izraba, piroliza, ostanki fermentacije, termogravimetrična analiza, gorivne lastnosti

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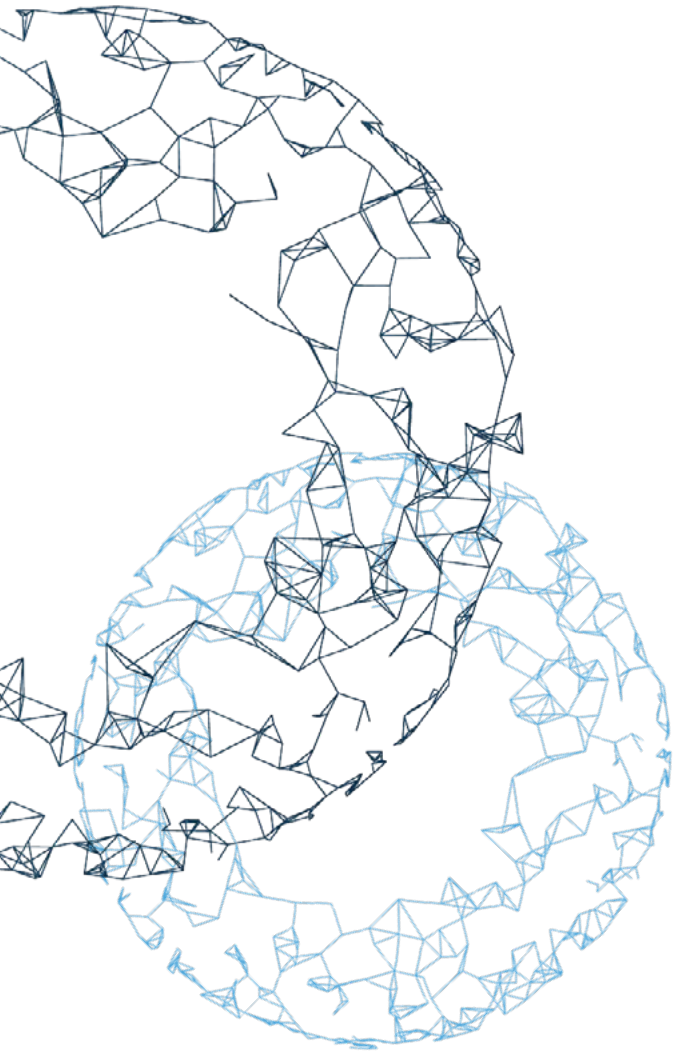

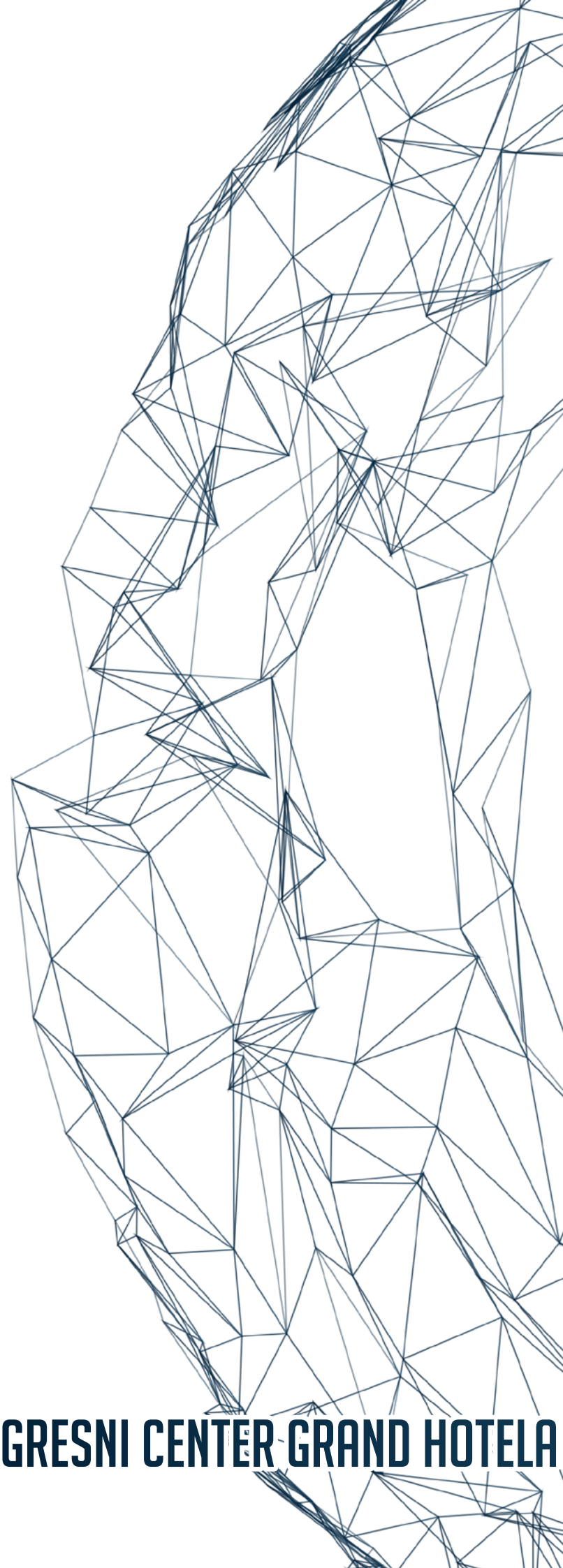

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