# Book of Abstracts

Jožef Stefan International Postgraduate School Students' Conference

17th Jožef Stefan
International Postgraduate
School Students' Conference

From Research to Reality

# *17th Jožef Stefan International Postgraduate School Students' Conference*

## *Book of abstracts*

*Edited by:*

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Publisher:
Jožef Stefan Institute & Jožef Stefan International Postgraduate School
28th – 30th May

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prof. dr. Milena Horvat – Ecotechnologies
dr. Nives Ogrinc – Ecotechnologies
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# IPS Student Council

This year, the conference returned to the beautiful town of Kamnik, nestled at the foot of the Kamnik–Savinja Alps. Surrounded by mountains and rich in history, the monastery provided an inspiring backdrop for our annual gathering. It was the perfect setting for this year's theme: *From Research to Reality*. We chose this theme with a clear purpose. Research, while exciting and often deeply technical, can sometimes feel distant from everyday life. But when we reflect on how our work can be applied, shared, and even commercialized, it gains new relevance. This conference was about exploring that journey—how ideas move from the lab to real-world impact.

Several invited talks explored this idea in different ways. Dr. Luka Suhadolnik from the National Institute of Chemistry and Quipnex shared how he combined academic research with entrepreneurship, offering insights from his startup experiences. Mag. Luka Radičević and mag. Neja Bizjak Štrus from the Young Academy of Slovenia highlighted how institutions can support young researchers and why entrepreneurial thinking matters. Assist. Prof. Dr. Kristina Žagar Soderžnik provided another angle, describing how real-world challenges influenced her work on portable electrochemical sensors. From industry, we had insightful contributions that further grounded our theme. Dr. Rok Grahek from Lek discussed "Genotoxic Nitrosamines in Drug Products," shedding light on their safety implications and analytical approaches. Mag. Nadja Kern Prezelj from Avantor presented featured solutions for advanced battery science, life sciences, and analytical chemistry—reminding us that many of our scientific problems are already knocking on industry's door. This year's round table brought together IPS alumni Dr. Rok Novak, Dr. Nina Kuzmić, and Dr. Ana Oberlintner. They reflected on their PhD journeys, the lessons learned, the challenges they faced, and their current career paths—highlighting both the personal and professional realities of research life.

Of course, the heart of the conference was—as always—the students. This year, we had 64 presentations from Master's and PhD students, covering everything from ecology to sensor technology, nanotech, and ICT. Each presentation was a reminder of how much exciting research is happening at IPS—and how much potential it has to make a real-world impact. This vibrant student-driven program was made possible thanks to the unwavering support of the Dean of IPS, Prof. Dr. Milena Horvat, and the dedication of the IPS staff—Prof. Dr. Aleksander Zidanšek, Sergeja Vogrinčič, and Tadeja Samec—as well as the efforts of the student organizing team, who's behind-the-scenes work ensured that everything ran smoothly from start to finish.

Finally, none of this would have been possible without the generous support of our sponsors. We sincerely thank the Jožef Stefan International Postgraduate School, the Jožef Stefan Institute, Ljubljana University Incubator, Avantor, Generali, Istrabenz plini, Lek, Chemass, Kolektor, Birdbuddy, Premogovnik Velenje, ELES, AciesBio, Anton Paar, Sanolabor, and Red Bull. Your continued support not only made it possible to organize this conference free of charge for all participants, but also helped us bridge the gap between science and practice—between research and reality.

We hope this year's conference sparked ideas, built new connections, and encouraged all of us to keep pushing our work one step closer to making a difference.

**Sebastian Mežnar, Anja Pavlovič, and Alnilan Lobato**
on behalf of the IPS Organizing Committee and the IPS Student Council

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## Foreword from the Dean

Each year, as the student conference of the Jožef Stefan International Postgraduate School approaches, we're given a rare and welcome opportunity to pause. To listen—not to ourselves, but to the voices of our students. Voices that rise from laboratories and fieldwork, from data models and discussions, from long hours of careful thought, and sometimes from doubt and quiet determination. This year especially, as we gather under the theme ***From Research to Reality***, those voices carry a deeper resonance.

This theme wasn't chosen by chance. At a time when the boundaries between science and everyday life are becoming increasingly fluid, it feels right to ask: how does knowledge move from theory to practice? How does it become part of something larger—a response to the climate crisis, a contribution to public health, or simply a better sensor, cleaner water, a more just system?

You can sense this movement in the contributions to this year's conference. Not just in the research excellence—measured in publications or project success—but in something more subtle: an inner commitment. A blend of curiosity, persistence, and a desire to make knowledge count. Many of you are already working with industry, involved in international collaborations, or actively seeking ways to turn your ideas into tangible outcomes.

But it's not just about results. It's about growth. This conference is as much a space for scientific content as it is a practice ground—for clarity, for communication, for listening to others. Often, the most meaningful moments arise after the talks, in the discussions—when a single thoughtful question opens up a whole new path of thinking.

I am grateful to all of you—students who step forward with your ideas, your openness, and your courage. And to the mentors, organizers, and all who shape this event—not as a formal obligation, but as a living conversation.

May your journey *from research to reality* remain a continuous one—guided by curiosity, shaped by reflection, and always open to new directions. This conference is just one stop along the way.

**Prof. Dr. Milena Horvat**
Dean of the Jožef Stefan International Postgraduate School

# Ecotechnologies

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# Increasing Efficiency of Biophotoelectrochemical Processes by Structuring Biofilms of Aerobic Phototrophic Microorganisms

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Biophotoelectrochemical (BPEC) systems harness the photosynthetic activity of microorganisms to generate electrical current and drive redox reactions, offering promising applications in renewable energy, biosensing, and wastewater treatment. However, practical implementation remains challenging due to long electrode maturation times, weak biofilm adhesion, and low electron transfer efficiency. To address these limitations, we investigate polyelectrolyte-assisted immobilization of *Chlorella sorokiniana* on electrode surfaces to enhance biofilm stability and conductivity. Polyelectrolytes facilitate biofilm formation by electrostatically binding cells to the electrode, potentially reducing maturation time from weeks to hours. We employed polyethyleneimine (PEI) to coat fluorine-doped tin oxide (FTO) glass, subsequently immobilizing *C. sorokiniana*. The biofilm formation was assessed using microscopy, while electrochemical performance was evaluated via cyclic voltammetry (CV) and chronoamperometry.

Preliminary results indicate successful attachment of microalgae to both FTO and carbon electrodes, with PEI-coated surfaces showing significantly improved coverage compared to unmodified electrodes. However, the generated electrical current remains below the detection limit of our potentiostat. These findings suggest that polyelectrolyte-assisted immobilization can improve biofilm formation and their longevity, but further optimization is required to enhance charge transfer. Future work will focus on increasing cell density and testing alternative conductive polymers to maximize BPEC system performance. This research contributes to the advancement of microbial electrochemical technologies, potentially accelerating their transition from laboratory research to real-world applications.

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# Reducing User Interaction Through Modular Platform Design: Enhancing Usability and Security

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Managing complex geospatial data processing often requires significant user interaction, creating barriers for domain- and technically-inexperienced users. This work addresses the human-computer interaction aspect of the challenge by designing and implementing a modular, plugin-based platform to streamline geospatial data workflows, significantly reducing cognitive and temporal loads on users - specifically, a local platform for the autonomous extraction of spatial data has been developed to preserve and protect sensitive information, particularly the privacy of location.

Initially, users faced difficulties using traditional R scripts due to high interaction demands and complex dependencies management. To mitigate these issues, a standalone, portable modular platform using independent plugins was selected, enabling flexibility, easier updates, and robustness, with minimal user intervention.

The platform simplifies the workflow by automating data retrieval, validation, storage, and processing tasks. Each plugin independently guides the user through specific tasks like data import, geospatial calculations, and output validation, further supported by minimalist UI principles that prevent user errors and enhance clarity. Security was integral, ensuring processes are secure by default and anonymization steps immutable by users.

Results demonstrate significant improvements in user experience and workflow efficiency, reducing complexity from multiple manual operations to just a few intuitive steps. The modular architecture allows seamless updates without interrupting user operations, providing adaptability for diverse future use-cases.

This work highlights the potential of thoughtful design of human-computer interaction in software development, achieving enhanced usability, flexibility, and security, crucial for supporting non-expert user engagement in scientific and technical contexts.

# Development of Analytical Method for Determination of Chemical Exposure Biomarkers in Hair

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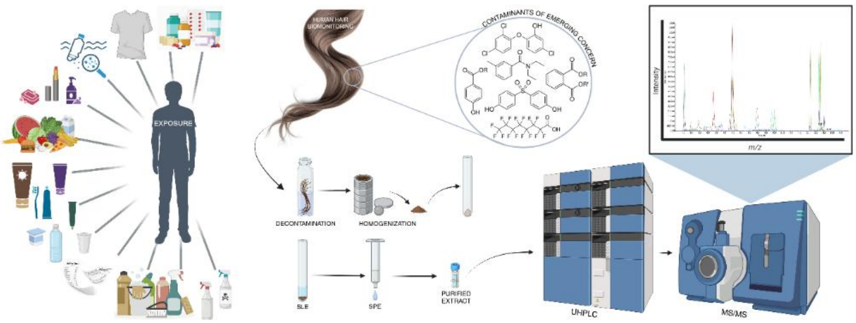

**Figure 1**: Determination of exposure biomarkers in hair.

Human exposure to contaminants of emerging concern is increasing due to industrial development and the widespread use of synthetic chemicals in consumer products and the environment. Biomonitoring environmental contaminants in human samples provides insights into exposure and its potential health effects. Traditionally, biomonitoring relies on matrices such as blood and urine, however, these are limited in assessing long-term exposure, especially for compounds with short biological half-lives. Hair presents an alternative, non-invasive matrix that offers a broader window of exposure assessment due to the accumulation of xenobiotics over time. Despite its potential, the application of hair analysis in biomonitoring is hindered by analytical challenges, gaps in knowledge regarding incorporation of biomarkers into hair and limitations in result interpretation.

This study focused on the development and validation of wide-range biomarkers of exposure (BoEs) in human hair samples. Hair was decontaminated first and homogenized using a ball mill. BoEs were extracted via solid-liquid extraction with methanol and ethyl acetate. Sample cleanup was performed using SPE HLB PRIME cartridges with a two-step pass-through protocol. Finally, the analysis was conducted using ultra-high-performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS) (Figure 1). The method validation involved matrix-matched calibration with background subtraction, and recovery assays, and demonstrated sufficient linearity and sensitivity, with limits of quantification ranging from 0.5 to 10 ng/g hair for most analytes. The suitability of the method was confirmed via analysis of 30 hair samples.

These findings support the use of hair as a viable matrix for biomonitoring specific BoEs, enabling a more comprehensive assessment of human exposure. The method developed in this study establishes a foundation for future research on hair matrix characteristics and untargeted screening approaches. This study represents the first biomonitoring of organic contaminants in hair in Slovenia, contributing to the advancement of exposure assessment using non-invasive matrices.

# The use of $^{50}$Cr(VI) and $^{53}$Cr(III) isotopic tracers in chromium speciation in mineral materials

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Cr(VI) compounds are highly toxic. To protect users of consumer products, the EU has restricted the marketing and use of Cr(VI) [1]. To meet regulatory requirements, it is important to determine Cr(VI) content in mineral materials. An analytical procedure for the determination of Cr(VI) in mineral materials is reported. Hot alkaline extraction was used to extract Cr(VI) from the sample. A 0.5 g of mineral material was weighed into glass beaker, and 45 mL of 2% NaOH + 3% $Na_2CO_3$ extraction solution was added. To prevent the oxidation of Cr(III) during extraction, 5 mL of 4 mol/L $MgCl_2$ was then added. The sample was transferred to an ultrasonic bath and sonicated for 30 min at 700 W and 90 °C, then cooled to room temperature, filtered (0.45 µm), and diluted 10 times with MilliQ water. Cr(VI) was determined in 10 times diluted extract by high performance liquid chromatography coupled to inductively coupled plasma mass spectrometry (HPLC-ICP-MS) at *m/z* 52, following the speciation procedure of Drinčić et al. [2]. To control for species interconversion during the extraction procedure, the sample was doubly spiked with enriched isotopic solutions of $^{50}$Cr(VI) and $^{53}$Cr(III) and, Cr(VI) was determined in 10 times diluted extracts at *m/z* 50, 52 and 53 [2]. The analytical procedure is highly sensitive with a LOD of 0.06 mg/kg, which is significantly below the regulatory requirements of EU legislation [1] that prohibits consumer products containing more than 2 mg/kg of Cr(VI). It is suitable for the analysis of Cr(VI) in mineral materials.

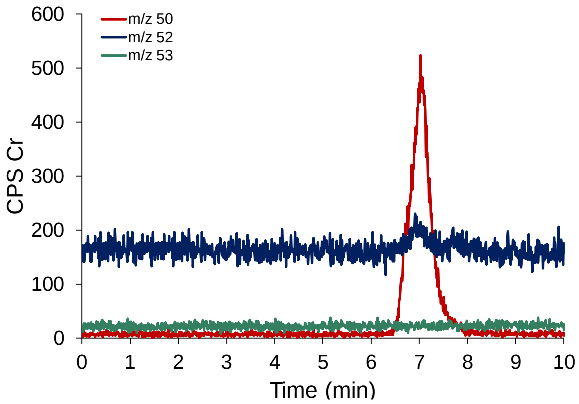

**Figure 1**. Chromatogram of Cr species in 10 times diluted alkaline extract of mineral material doubly spiked with $^{50}$Cr(VI) and $^{53}$Cr(III) (5 ng/mL Cr) by HPLC-ICP-MS, recorded at *m/z* 50, 52 and 53.

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# Spatial Structuring of Microbial Communities for Bioelectrogenically Stimulated Pollutant Degradation

Kristjan Gašpirc[1], Dmitrii Deev[1], Maja Zugan[1], Tayebeh Sharifi[1], Tomaž Rijavec[1] and Aleš Lapanje[1]*

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Effective bioremediation of pollutants is often constrained by our limited understanding of microbial spatial organization and niche formation. Spatial organization enables microbial interactions and formation of diverse microenvironments as a result of microbial activities. Engineered microbial communities, structured as biofilms or aggregates, provide practical ways to manage niche formation, which are essential for microbial growth and interactions. This approach holds potential, as it enables the cultivation of microbes that are challenging to grow individually because they depend on interactions with other species and may enhance pollutant degradation through bacterial cooperation.

We developed methods for the spatial distribution of cells and microgeographic structuring of microbial communities by optimally placing microbes within micrometer-scale proximity to promote effective interactions. Here, we performed preliminary experiments to evaluate a method for improving bacterial attachment on electrodes within a microbial fuel cell (MFC) system, using electropolymerization of pyrrole using the cyclic voltammetry technique on graphite electrodes. Confocal fluorescence microscopy was used to visualize and quantify bacterial attachment and the formation of artificial biofilms on the electrode surface.

Our results show enhanced immobilization of the electrogenic bacterium *Shewanella oneidensis* MR-1 on graphite electrodes. Preliminary findings indicate that after 14 days of incubation, bacterial presence was higher on polymer-coated electrodes compared to uncoated control electrodes.

Ultimately, this research shows a first step towards forming a multilayered biofilm that can act more effective in transformation and pollutant degradation in biolectrogenically supported bioremediation. These results provide a good starting point for future work in improving bioremediation processes.

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# Air pollution by Polycyclic Aromatic Hydrocarbons (PAHs) in Europe and Slovenia: A Modelling Approach

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Polycyclic Aromatic Hydrocarbons (PAHs) are toxic organic compounds released into the environment through the incomplete combustion of fossil fuels and biofuels. Many PAHs are carcinogenic, mutagenic, and teratogenic, posing risks to human health and ecosystems. Human exposure occurs via inhalation, dermal contact, or ingestion of contaminated food. While PAH air concentrations in Europe have declined considerably over the past decades, further reductions have stalled, keeping population exposure a concern.

This study examines PAH air pollution in Europe, with a focus on Slovenia, analyzing current levels, geographical distribution, and source attribution of PAH concentrations in ambient air. The chemical transport model GLEMOS was used to simulate the atmospheric dispersion of selected PAHs from emissions across Europe. The model accounts for various environmental processes, including atmospheric transport, chemical transformation, deposition, accumulation in soil, water, and vegetation, and re-emission.

The results indicate elevated PAH concentrations in Central, Southern, and Eastern Europe with annual mean benzo[a]pyrene (B[a]P) levels in several countries exceed the EU target value of 1 ng/m$^3$ (Directive 2004/107/EC), posing potential health risks. In Slovenia, elevated annual mean B[a]P concentrations above 0.5 ng/m$^3$ are observed near major cities (Ljubljana, Maribor) and in the eastern part of the country with strong seasonal variation with much higher levels in winter. On average, national emissions contribute about 60% of B[a]P air concentrations, with residential combustion being the dominant source, particularly in urban areas.

These findings underscore that PAH pollution remains a pressing issue in Europe, despite past regulatory successes. The integration of high-resolution modelling with targeted measurement data is crucial for identifying key pollution sources and supporting evidence-based policy actions. In Slovenia and beyond, reducing residential combustion emissions could offer one of the most impactful routes for achieving cleaner air and protecting public health.

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# Electrochemical Analysis of the Influence of Surface-Active Substance on Surface Tension and Gas-to-Particle Mass Transfer

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Atmospheric aerosol particles are a crucial component of the atmosphere. They affect visibility, human health, and the global climate by enabling cloud formation, altering precipitation, and influencing the Earth's radiation balance. Their complex composition varies depending on the size, the time of day, and their source. One of the major constituents of atmospheric aerosol particles is the organic fraction, with a significant portion representing surface-active substances (SAS). Because of the presence of both hydrophobic and hydrophilic elements in their structure, SAS tend to partition to the gas-water interface and alter the surface tension of the particles, usually decreasing it. This decrease facilitates gas-to-particle transport, enhancing particle formation, hygroscopic growth, and affects cloud formation. [1,2]

Measuring this decrease is crucial in understanding the effects of SAS on atmospheric aerosol particles. In this research, we used a new electrochemical approach to study changes in surface tension caused by the presence of short-chain carboxylic acids (lactic, hexanoic, succinic) commonly found in atmospheric aerosol samples. As an alternative to conventionally used tensiometric methods (i.e. pendant drop), electrochemical tensiometry represents a more reliable and sensitive method for measuring changes in surface tension. With it, it is possible to measure changes in surface tension even at significantly lower and more atmospherically relevant concentrations compared to standard techniques. [3]

Further, the influence of carboxylic acids on the rate of the gas-to-particle mass transfer of different volatile compounds (bromoform, naphthalene, and pyrene) was investigated. The results show the potential role of SAS in enhancing the gas-to-particle mass transfer, which can influence atmospheric particle growth and the particle's heterogeneous chemistry.

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# The Role of Water-Insoluble Organic Carbon (WIOC) in Atmospheric Particles and Its Impact on Climate

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Due to their limited predictability, the uncertainties in estimates of radiative forcing by atmospheric aerosols are the largest among all other agents, including greenhouse gases. This arises from the unknown sources of secondary-produced forcing agents, constituting a significant fraction of atmospheric aerosols. Organic carbon, as a significant component of atmospheric aerosol particles, plays a crucial role in radiative forcing due to its high reactivity and contribution as a newly recognized light-absorbing agent. Each reaction with the potential to produce light-absorbing chromophores acts as a source. Therefore, relevant reactions and mechanisms must be identified to accurately understand and predict their influence on climate, which remains challenging. Extensive research has been conducted on light-absorbing water-soluble organic carbon (WSOC). However, water-insoluble organic carbon (WIOC), although present in a smaller fraction of organic carbon mass, absorbs light more efficiently and can have an even bigger impact on the climate.

Optical properties of atmospheric aerosol particles are typically determined using various spectrophotometric techniques. While some of these techniques determine the absorption properties of single particles and others of bulk-collected particles, such approaches enable the classification of various compounds present in atmospheric particles into distinct groups. Chromatography and mass spectrometry are effective for the chemical characterization of individual compounds within each classified group. Despite state-of-the-art instruments for analyzing WIOC compounds, challenges persist, making it difficult to fully understand atmospheric particle composition and their influence on the climate.

In my PhD work, I will focus on synergistically combining extraction, ionization, chromatographic, mass spectrometric and other analytical techniques, to tackle the above-mentioned challenges and to improve the resolution of analytical methodologies, with the intention to ensure the proper quantification and determination of WIOC species.

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# Synthesis and characterization of monomeric $[PhC(NtBu)_2]SiCl$ with Selenium and Tellurium

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Low-valent silicon compounds represent an important class of substances with high chemical reactivity. One of the key representatives of this class is the amidinate silylene LSiR (L = $PhC(NtBu)_2$, R = a halide or an organic substituent). Its structure enables unique interaction mechanisms, making it a promising reagent for small molecule activation and novel chemical transformations [1].

Indeed, the reactions of LSiR with various compounds have been extensively studied, including its interactions with alkynes, chalcogens, ketones, carbon monoxide, and $P_4$ [2, 3]. However, studies on the reactivity of these compounds with chalcogens have mainly focused on the interactions of LSiR (R = halide) with sulfur [1], while reactions with selenium and tellurium remain poorly explored.

In this regard, the aim of this study is the synthesis of monomeric compounds $[PhC(NtBu)_2]SiCl{=}Se$ and $[PhC(NtBu)_2]SiCl{=}Te$. To obtain them, we optimized stoichiometry, solvent selection, and temperature control. The synthesized compounds were characterized using $^{1}H$ and $^{77}Se$ NMR spectroscopy, as well as single-crystal X-ray diffraction, confirming their monomeric nature.

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# Fate of polystyrene nanoplastics and potentially toxic elements in hydroponically grown tomato plants

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Reusing treated wastewater for plant irrigation presents a sustainable solution to water scarcity, however, the risks associated with contaminant uptake in edible plants remain unknown. Nanoplastics (NPs), ubiquitous in all environmental compartments, pose a significant concern due to their size, allowing them to penetrate plant tissues. Additionally, NPs can influence the mobility and bioavailability of other pollutants, such as heavy metals. To fully assess the risks posed by NPs along with other potentially toxic elements (PTEs) in the human food chain, quantitative research on their uptake and translocation is essential.

In this study, hydroponically grown tomato plants were exposed to polystyrene NPs doped with europium (PS-Eu NPs, 200 nm, 1 mg/L), either alone or in combination with isotopically enriched elements: $^{53}$Cr, $^{70}$Zn, and $^{204}$Pb (0.1 mg/L), and $^{106}$Cd (0.05 mg/L). After five weeks of exposure, harvested plant samples (roots, stems, leaves, fruits) were analysed using ICP-MS. The stability of Eu in PS-Eu NPs was assessed under exposure conditions to accurately use Eu as a proxy for NPs.

The results showed that Eu was detected in all parts of the tomato plant, with the highest concentrations in roots, followed by leaves, stems, and fruits. Considering the 4% leaching of Eu in medium simulating plant cell environment, it remains unclear whether the low concentrations of Eu found in fruits result from PS-Eu NP uptake or dissolved Eu leached from PS-Eu NPs. The presence of PS-Eu NPs influenced the uptake and distribution of PTEs, with no impact on Cd and Zn concentrations, but a decrease in Cr and Pb levels, likely due to steric effects, their adsorption on NPs, and/or precipitation. Consuming tomatoes grown under hydroponic conditions could lead to intake of toxic elements, including cadmium (Cd), and pose potential health risks, while the adverse effects of NPs remain to be confirmed.

# Synthesis and Characterization of Coordination Compounds $[M(XeF_2)_n](AF_6)_2$ ($M = Cu, Ni$; $A = Ru$)

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In 1962 Neil Bartlett synthesized the first noble gas compound, $XePtF_6$ [1]. Less than a year later, $XeF_2$ was synthesized [2]. $XeF_2$ can act as a ligand, coordinating to metal cations. The first synthesized compound of this type was $[Ag(XeF_2)_2]AsF_6$ [3]. Since then, numerous compounds with the general formula $[M(XeF_2)_n](AF_6)_m$ have been synthesized, where "n" is the number of coordinated $XeF_2$ molecules, "m" is the oxidation state of the metal cation M, and $AF_6$ represents a weakly coordinating anion (WCA) formed from Lewis acids like $SbF_5$, $AsF_5$, $BiF_5$ [4]. The goal of the PhD research is to synthesize compounds in which the $XeF_2$ molecules coordinate to a metal cation, with a weakly coordinating anion (WCA) serving as the counterion. Initial characterization of synthesized compounds is performed via Raman spectroscopy, providing first insights into the structure and composition. This is followed by the preparation of crystals and the determination of the crystal structure using X-ray diffraction of single crystals. Several new coordination compounds with Cu(II) and Ni(II) as metal centers using $RuF_6^-$ as a WCA have been synthesized: $[Cu(XeF_2)_2](RuF_6)_2$, $[Ni(XeF_2)_2](RuF_6)_2$ (Figure 1), $[Cu(XeF_2)_6](RuF_6)_2$, and $[Ni(XeF_2)_6](RuF_6)_2$. We want to expand knowledge on $XeF_2$-coordinated metal complexes by varying metal cations and WCAs, providing deeper insight into their structural and chemical properties.

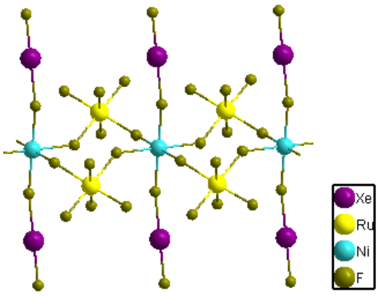

**Figure 1.** A part of the infinite chain of $[Ni(XeF_2)_2](RuF_6)_2$.

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# Immunomodulatory and Toxic Effects of Aluminium Fluoride Complexes on Macrophages

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Aluminium fluoride complexes ($AlF_x$), which form in the presence of fluoride ($F^-$) and aluminium (Al), are known to affect protein phosphorylation through G-protein mimicry [1]. While their theoretical mechanism is well described, *in vitro* studies remain scarce. This study aimed to evaluate and compare the toxicity and immunomodulatory effects of $F^-$, Al and $AlF_x$ using a THP-1 macrophage *in vitro* model. Macrophages were treated with standard solutions of $F^-$, Al or $AlF_x$ (2–2000 μM). Cell viability was assessed using the Propidium Iodide/Annexin V assay after 48 hours, while inflammatory cytokine levels were measured after 24 hours using the multiplex assay Legendplex Human Inflammation Panel 1. Our results indicate that $F^-$ exhibited the highest cytotoxicity, whereas Al and $AlF_x$ were less toxic. The $AlF_x$ complexes showed the strongest immunostimulatory effects, inducing the highest levels of inflammatory cytokines. The low toxicity of $AlF_x$ in combination with strong immunomodulatory effects suggests their potential as vaccine adjuvants.

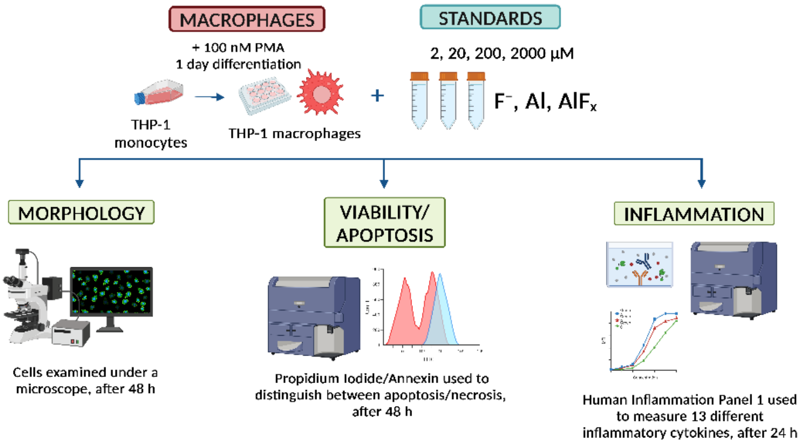

**Figure 1**. Schematic representation of the methods used in our study.

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# Integrating GC-MSD and GC-C-IRMS for Fatty Acid Profiling: Assessing Quality Differences Between Wild and Farmed Seabream

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The growing focus on healthy eating has increased interest in the nutritional benefits of fish, particularly their high ω-3 polyunsaturated fatty acid (PUFA) content. Additionally, consumers are becoming more concerned with product authenticity, highlighting the importance of accurate labeling regarding production methods and origin. The simultaneous use of fatty acid profiling and stable isotope approach can provide complementary evidence to distinguish between food sources and substantiate the dietary preferences of marine organisms, that would otherwise be obtained from one technique alone. This study presents a comprehensive approach to analyzing the seabream fatty acid profile, first by assessing fatty acid composition using Gas Chromatography-Mass Spectrometry Detection (GC-MSD) and second by determining carbon stable isotope of individual fatty acids using Gas Chromatography-Combustion Isotope Ratio Mass Spectrometry (GC-C-IRMS) for quality evaluation. The most important PUFAs for physiological function—linoleic acid (LIN; 18:2n-6), alpha-linolenic acid (ALA; 18:3n-3), eicosapentaenoic acid (EPA; 20:5n-3), and docosahexaenoic acid (DHA; 22:6n-3)—may be especially useful in tracing dietary sources. Sample collection was conducted over a one-year period, from July of 2023 to March of 2024, and included 163 seabream samples from the Mediterranean Sea, Atlantic Ocean and Adriatic Sea. Authentic seabream samples from Malta, Spain, and Portugal, included both wild-caught and farmed fish, while commercial samples from Slovenia and Croatia, were exclusively farmed.

We found significant differences in fatty acid profiles between wild and farmed seabream, with the most prominent in EPA (7.4%) and DHA (17.1%) in wild fish, compared to 2.1% and 5.3% in farmed seabream, respectively. These variations are influenced by factors such as diet, environmental conditions, geographical location, production method, species, etc. Additionally, we anticipate variations in carbon isotopic signatures of individual fatty acids among seabream samples, providing further insights into their biogenetic, but also origin of production. Overall, this study underscores the effectiveness of combining fatty acid profiling and stable isotope analysis to differentiate between wild and farmed seabream, providing valuable insights into their feeding patterns and overall quality.

# Urban Cycling Lab: citizen science protocol to assess and reduce cyclists' exposure to environmental stressors

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Bike commuters are exposed to various environmental factors that cumulatively impact their health and well-being. The Urban Cycling Lab is designed as a citizen science intervention to evaluate bike commuters' exposure to environmental stressors—specifically particulate matter (PM) and noise—while promoting route choices that minimize exposure (Figure 1). Grounded in behavior change theory, the study leverages a sensor-enhanced ICT infrastructure to support citizen engagement. Participants use personal biometric and environmental sensing devices alongside the project-build web app *(Primerjlanik.si)* to compare geo-coded real-time exposure levels across different routes. Additionally, the exposure assessment includes (bio)chemical analysis of blood and urine. To understand how bike commuters perceive and select their routes, ride-along interviews are conducted, exploring awareness of environmental exposure and opportunities to reduce exposure. By integrating technology-driven user involvement and co-creation processes, this study aims to explore the potential of citizen science in gathering evidence related to environmental stressors, while simultaneously influencing cyclists' route choices and advocating for environmentally-conscious urban planning.

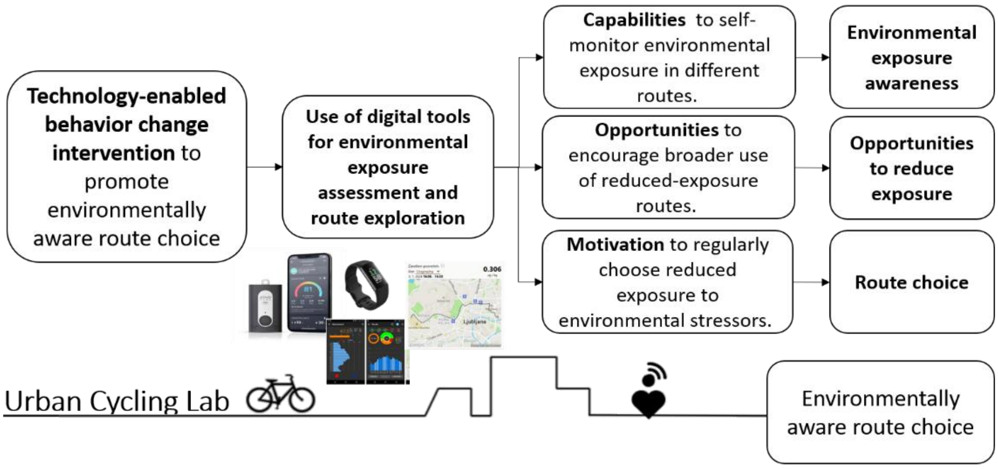

**Figure 1**. The Urban Cycling Lab was designed as a theory-driven, technology-enabled citizen science intervention.

# Edible Oils from Synthesis to Waste: A Stable Isotope Approach

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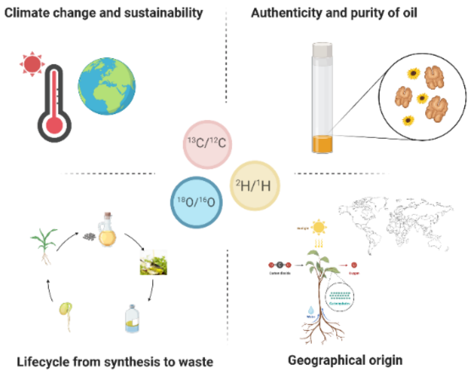

**Figure 1** Graphic abstract

In recent years, the consumption of edible vegetable oils has significantly increased. While palm oil, soybean oil and rapeseed oil remain the most widely produced and consumed, there is a growing interest in high-value specialty oils. A similar trend has been observed in Slovenian market, where oils such as walnut oil, grape seed oil, poppy seed oil, hemp oil, hazelnut oil, castor oil, apricot seed oil, avocado oil and primrose oil are increasingly present on retail shelves, reflecting a shift in consumer preferences toward diverse and nutritionally rich oil sources. Due to their beneficial effects on human health and high market price, these oils are often susceptible to adulteration, highlighting the critical need for reliable authentication and traceability methods to ensure quality, safety, and consumer trust. This study explores the potential of stable isotope analysis as a powerful tool for verifying oil authenticity and tracing its production from synthesis to waste quality control. Stable isotope ratio analysis of key elements such as carbon, hydrogen, and oxygen provide valuable insights into authenticity and traceability of oil, it's metabolic pathways, isotopic fractionation as well as environmental influences and waste oil management (Figure 1). Furthermore, the identification of specific biomarkers and their isotope signatures enhances the detection of adulteration. While stable isotope techniques offer high precision and accuracy, their integration with complementary methods such as volatile organic compound (VOC) profiling, fatty acid composition analysis, and elemental analysis further strengthens quality assurance and food fraud prevention. By combining advanced analytical techniques, this study underscores the importance of a multidimensional approach to ensuring the authenticity, safety, and sustainability of newly marketed high-value oils to protect them against adulteration. Additionally, by studying metabolic pathways and the fractionation of stable isotopes, we seek to better understand the effects of environmental factors on oil composition.

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# Lifestyle, geospatial and genetic factors impacting urinary metabolites of polycyclic aromatic hydrocarbon in Slovene children

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Polycyclic aromatic hydrocarbons (PAHs) are a group of compounds containing two or more aromatic benzo rings fused together. They are typically chemically inert, however upon entering the organism they can become highly reactive and harmful through metabolic activation. The most recent population survey data on PAH exposure include data from the European human Biomonitoring Initiative (HBM4EU) and the first national human biomonitoring programme in Slovenia (SLO-HBM-I). Notably, use of the exposure load method on the data from the latter programme has shown PAHs to significantly contribute to chemical exposure from the environment. However, both studies only include adults, the first study doesn't include participants from Slovenia and the second study used samples collected over a decade ago. This study utilizes participants of the second national human biomonitoring programme in Slovenia (SLO-HBM-II), which focuses on primary school children. Eleven PAH analytes representing 5 parent compounds were measured in urine samples collected between 2018 and 2024. Extensive demographic, health- and lifestyle-related data were also collected using questionnaires. The statistical analysis performed on the sum of analytes will include calculating basic statistical parameters, examining potential age-, sex and area-based differences and connections to other demographic and lifestyle-related factors. In addition, the potential impact of various environmental factors (e.g. ambient air concentrations, traffic intensity) and genotypes for selected enzymes involved in PAH metabolism were examined. This study is expected to not only provide an update on the existing data regarding PAH exposure, but also expand it to include a vulnerable demographic group previously uncharacterised in Slovenia.

# Integrating Stable Isotope Profiling, Multi-Elemental Analysis, and Statistical Modeling for Saffron Origin Authentication and Traceability

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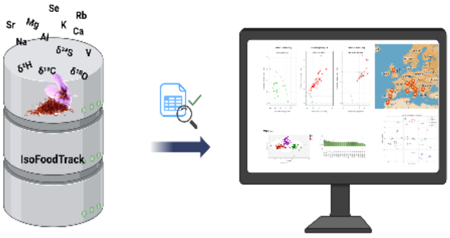

**Figure 1.** Graphical Abstract

Saffron, often referred to as 'red gold,' is one of the world's most valuable spices, making it a prime target for food fraud, including adulteration, mislabeling, and false origin claims. Its high market value, labor-intensive cultivation, and sensitivity to environmental factors create significant challenges in ensuring its authenticity and traceability. This study addresses these challenges by employing innovative analytical techniques, including stable isotope profiling and multi-elemental analysis, alongside advanced statistical modeling. A total of 201 saffron samples (163 authentic) were used in this study, integrating data from two previous studies—Perini et al. (2020) and Wakefield et al. (2019) [1,2] which employed similar approaches and methodologies, as well as 75 newly collected samples (48 authentic) from Morocco, Greece, Slovenia, Spain, Iran, and the United Kingdom. These 75 samples were analyzed using Isotope Ratio Mass Spectrometry (IRMS) and Inductively Coupled Plasma Triple Quadrupole Mass Spectrometry (ICP-QQQ). All data are compiled within the IsoFoodTrack database [3]. Discriminant analysis (OPLS-DA) of the data enabled saffron origin classification with 94% accuracy. Key discriminatory markers included $\delta^{2}$H, $\delta^{15}$N, K, Ca, $\delta^{13}$C, Sr, Mn, Co, and Zn. The integration of elemental ratios (Rb/Sr, K/Rb, Ca/Sr) and $\delta^{18}$O further enhanced geographical differentiation. Verification of saffron labeling with a DD-SIMCA classification model revealed potential mislabeling in up to 60% of samples, highlighting the need for improved authentication measures. A new approach using Explainable Artificial Intelligence (XAI) is being developed to enhance saffron authentication by revealing key variables driving model decisions and improving transparency in the process. While saffron was used as a case study, this methodology is adaptable for other food commodities, offering a scalable solution to combat food fraud along the supply chain.

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Acknowledgments

We acknowledge the financial assistance of the FoodTraNet Project funded by the European Union's Horizon 2020 research and innovation programme under the MSCA Grant agreement No. 956265 and PROMEDLIFE project (PRIMA programme supported by the European Union | Grant agreement No. 2132). Some samples were collected as part of an IAEA funded CRP D52042: "Implementation of Nuclear Techniques for Authentication of Foods with High-Value Labelling Claims (INTACT Food)".

# The Role of Carbonation Timing on Alkali-Activated Materials

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The construction sector is a major contributor to global emissions. With increasing regulatory pressure, industries that rely on $CO^2$-intensive processes must move towards sustainable practices. Alkali-activated materials (AAMs) provide an environmentally friendly alternative to cement by valorizing industrial by-products such as slag, ash and clays. In addition, $CO^2$ sequestration in calcium-rich waste materials, such as biomass ashes, allows $CO^2$ to be permanently bound in mineral carbonates, thereby reducing the industrial carbon footprint.

The study investigates the influence of carbonation timing on AAMs. Highly porous AAMs were produced from biomass ash and exposed to various curing conditions including ambient, high-temperature and humidity, and elevated $CO^2$ levels. Emphasis was placed on comparing carbonation during AAM curing with delayed carbonation applied after curing. The effects on mechanical properties, microstructure and chemistry of AAM were assessed using mercury intrusion porosimetry (MIP), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy with energy dispersive spectroscopy (SEM-EXDS). Results indicate that premature carbonation interferes with the development of the AAM matrix by restricting Ca availability, leading to increased porosity and reduced mechanical properties. Conversely, delayed carbonation, introduced after AAM curing, resulted in well-developed mechanical properties comparable to those achieved with high-temperature and humidity curing. XRD and SEM-EXDS analysis confirmed the presence of Ca-carbonates in the pores of carbonated samples.

The research highlights $CO^2$ sequestration as an innovative approach to sustainable building materials. However, precise control of carbonation timing and conditions is essential to maximize the environmental benefits of $CO^2$-induced mineralization without compromising material performance.

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# Quantifying the Seasonal Influence of Building Air Infiltration on Indoor and Outdoor $PM_{2.5}$ Distributions

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The airtightness of a building envelope plays a crucial role in regulating the transport of air and pollutants into and out of the indoor spaces. This case study investigates a naturally ventilated one-bedroom apartment in central Slovenia, focusing on the evaluation of air infiltration rates through the building envelope under various meteorological conditions at daily and seasonal scales and the relationship between outdoor and indoor $PM_{2.5}$ concentrations.

Air infiltration rates ($N_{inf}$ [$h^{-1}$]) were determined using the $CO_2$ tracer gas method in an unoccupied space. Simultaneously, indoor and outdoor $PM_{2.5}$ concentrations, along with meteorological parameters (including air temperature, air pressure, relative humidity, wind speed, and precipitation), were continuously monitored during winter, spring, and summer.

The results revealed distinct seasonal variations in $N_{inf}$: winter 0.15–0.58 $h^{-1}$ (mean: 0.30±0.08 $h^{-1}$), spring 0.18–1.39 $h^{-1}$ (mean: 0.38±0.26 $h^{-1}$), summer 0.10–2.92 $h^{-1}$ (mean: 0.55±0.61 $h^{-1}$). Corresponding indoor-to-outdoor $PM_{2.5}$ ratios also varied: winter 0.43–2.20 (mean: 1.10±0.46), spring 1.02–10.4 (mean: 2.6±2.2), summer: 0.30–1.90 (mean: 0.88 ±0.39). Among all meteorological parameters, the indoor-outdoor temperature difference exhibited the strongest correlation with $N_{inf}$ across seasons.

Understanding these dynamics is essential for optimising building envelope design and ventilation strategies aimed at maintaining indoor air quality.

Acknowledgements

Slovenian Research and Innovation Agency (research core funding No. P2-0158, Structural engineering and building physics; No. P1-0143, Cycling of substances in the environment, mass balances, modelling of environmental processes and risk assessment).

# Information and Communication Technologies

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# Fine-Tuning Large Language Models for Medical Information Extraction from Hospital Records

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Hospitals frequently store patient visit and surgical operation data in unstructured textual formats, making it difficult to extract and structure relevant medical information. Manual extraction of information is time-consuming, diverting medical staff resources from other clinical duties. To automate and enhance the efficiency of medical information extraction, we evaluated several Large Language Models (LLMs) utilizing three distinct methodologies: prompt-only (zero-shot), few-shot prompting, and model fine-tuning.

The **prompt-only** approach evaluates a model's inherent capability to perform information extraction task without additional training or examples, relying solely on instructions within the prompt. The **few-shot prompting** in our approach provides the model with three labeled examples within the prompt, allowing it to adapt and perform better without training. In contrast, the **fine-tuning** approach involves additional training on annotated datasets, optimizing the model specifically for medical information extraction.

As a performance baseline, we fine-tuned GLiNER, a named entity recognition model leveraging a bidirectional transformer encoder architecture, on the same dataset used for fine-tuning the LLM models. Model performance was assessed using the F1 score, the harmonic mean of precision and recall. Our findings revealed that the prompt-only approach struggled to follow the required output structure, making information extraction infeasible. The few-shot prompting approach produced the desired output structure but performed poorly overall, correctly extracting only the most obvious entities and failing on more specific ones. In contrast, fine-tuned LLM models showed significant improvements in overall performance, surpassing GLiNER across all entity categories, particularly excelling at identifying less common entities.

Our results indicate that fine-tuning LLMs represents the most effective method for extracting structured medical information from clinical records.

**Acknowledgments**

This work was supported by the Slovenian Research Agency, and the European Union’s Horizon project PREPARE [grant number 101080288].

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# Product Quality Explorer - determining product quality based on the digital product passport

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The use of recycled materials in manufacturing industries is steadily increasing. Because recycled materials bring more impurities into the finished products, manufacturers must be more thorough in performing product quality control. Currently, they must manually inspect each finished product, which is both economically and time-inefficient.

Our research aims to solve this problem by predicting the quality of the products from the digital product passport data, so manufacturers wouldn't have to manually test for defective products. To achieve this, we are developing a user-friendly software system with a graphical interface designed to guide users without programming expertise through data analysis and predictive analytics. Our approach integrates multiple machine learning algorithms (logistic regression, decision trees, random forests, gradient boosting, SVM, and MLP) with genetic algorithms for attribute selection optimization and explainable AI techniques for model interpretation. The system is being tested on data from carbon fibre reinforced polymer (CFRP) manufacturing and other open databases.

Expected outcomes are also the identification of key quality factors and production process insights. The results should confirm that digital product passports can effectively support quality prediction models, enabling better decision-making in manufacturing and reducing waste through improved lifecycle management. We also aim to advance circular economy principles by helping manufacturers understand which materials can be reused and which must be discarded before going into production.

## Acknowledgments

This work was supported by the Slovenian Research Agency, and the European Union's Horizon project PLOOTO [grant number 101092008].

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# Sequential DAG Generation

**Job Petrovčič[1]*, Sebastian Mežnar[1,2], Ljupčo Todorovski[1,2]**

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Generating graphs is a fundamental task across various research fields. Given the exponential complexity of the graph space, statistical methods can help streamline the search process [1].

In this work, we focus on the generation of a special class of graphs: rooted directed acyclic graphs (DAGs) with ordered children. Mathematical expressions fall into this category, as they are represented by abstract syntax trees, which can be compressed into DAGs by merging identical subtrees.

We frame the rooted tree generation task as a sequential process where nodes are generated in the context of previously generated nodes, following [2]. We extend this approach to generate rooted DAGs using phantom nodes. During generation, connections are determined based on the dot product similarity between the embeddings of the phantom and already generated nodes.

We adapt the transformer architecture to capture the node context, while the graph structure is encoded using additional learnt embeddings. We evaluate our method on generating expressions in the proof assistant Lean 4. Our results show that this adaptation outperforms recurrent neural networks (RNN) in generating abstract syntax DAGs for mathematical expressions.

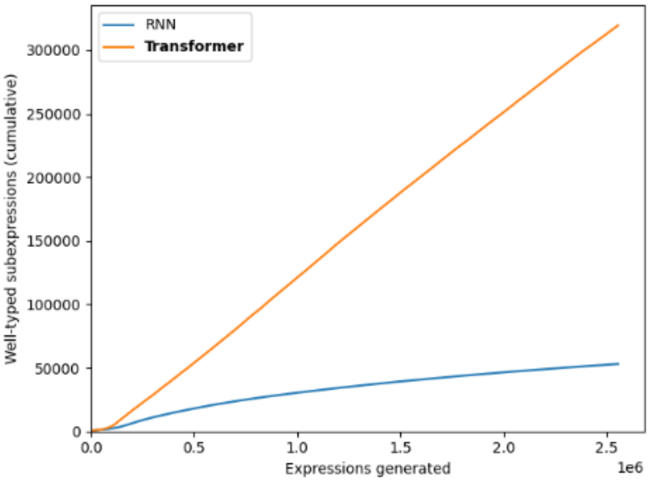

**Figure 1**. Graph showing that the adapted transformer outperforms RNN in the task of finding new (sub)expressions.

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# A Multimodal Approach to Predicting Cognitive Load

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Psychological constructs include complex behavioral patterns and experiences that are not directly observable. In psychology, these constructs are usually measured using self-reports, behavioral observations, and physiological signals [1]. While self-report methods are widely used, they require active participation from respondents. In our research, we addressed this challenge by using unobtrusive sensors, namely a regular camera, thermal camera, and eye-tracker to monitor 19 participants during a battery of tests for inducing cognitive load. The classification problem involved three target classes: 'low cognitive load,' 'high cognitive load,' and 'questionnaire'. Among the tested algorithms, Random Forest (RF) demonstrated the best performace in our leave-one-subject-out cross-validation, reaching an average F1-score of 0.45 across subjects, compared to an average baseline F1-score of 0.27. Accuracy of RF is illustrated in Figure 1. Additionally, our analysis of feature importance revealed that thermal-camera-derived features were the most informative. Our findings indicate that psychological states such as cognitive load can be predicted using unobtrusive sensors, but the methodology needs to be refined for improved accuracy.

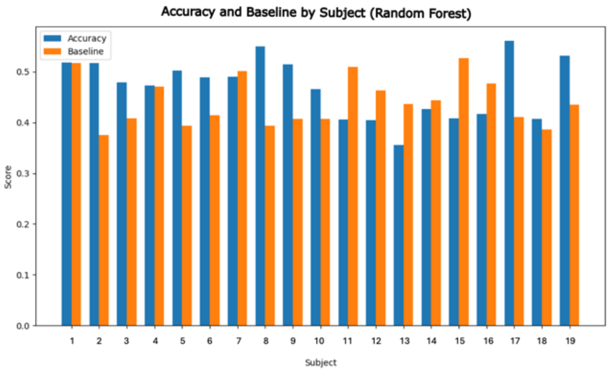

**Figure 1**. Accuracy and Baseline by Subject (Random Forest).

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Acknowledgement

I sincerely thank my colleagues for their assistance in data collection and preprocessing.

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# Discovery of exact equations via computing Gröbner basis

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Our work addresses the task of equation discovery, i.e., identifying equations that describe relationships within given data. In contrast with traditional equation discovery, which finds approximate equations from noisy measurements, we focus on discovering exact equations from noise-free data. We reformulate the equation discovery task into computing the Gröbner basis of a vanishing ideal in algebraic geometry. Using the algorithms for computing the Gröbner basis, we design and implement MoadeeB, a new algorithm for discovering exact equations from data. We evaluate MoadeeB on discovering recursive equations for more than 30,000 integer sequences from the Online Encyclopedia of Integer Sequences (OEIS). The evaluation results show that MoadeeB performs better than state-of-the-art algorithms for equation discovery and code synthesis in terms of reconstruction of existing and discovery of new equations (Table 1). The findings indicate a promising future for Möller-Buchberger algorithm-based methods in equation discovery, applicable to both exact and numerical data.

| OEIS ID | Discovered equation |
|---|---|
| A001699 | $a_n = -a_{n-2}^3 + a_{n-1}^2 + 3a_{n-1}a_{n-2} + 2a_{n-2}^2 + 2a_{n-1} - 4a_{n-2}$ |
| A002658 | $a_n = -(a_{n-2}^3 - 2a_{n-1}^2 - 6a_{n-1}a_{n-2} - 4a_{n-2}^2 - 8a_{n-1} + 11a_{n-2})/4$ |

**Table 1**. Two newly conjectured equations, discovered by MoadeeB, were subsequently approved by the OEIS curators and added to the encyclopedia. The equations were verified on the first 20 sequence terms (the 13th term contains 725 digits) and the first 25 sequence terms (the 18th term contains 12,521 digits) for the sequences in the second and third rows, respectively.

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# Improving Robot Cloth Unfolding with Basic Motion Heuristics

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Cloth unfolding is a prerequisite action for most cloth manipulation tasks. Its importance has led to the development of a benchmark and a competition on cloth unfolding using the *Regrasping in the Air strategy*, which took place at the 2024 IEEE International Conference on Robotics and Automation (ICRA). While the competition was conducted on a common dual-arm robot configuration composed of two UR5e robots with 6 degrees of freedom (DOF), recreating it with different robot arms to develop and test algorithms has led to hardware-specific issues and solutions.

We replicated the ICRA 2024 Cloth Competition setup using two 7-DOF Franka Emika FR3 robots and implemented a grasp selection and execution framework for dual-arm cloth unfolding based on the framework provided by the organizers. However, differences in the kinematic structures of the UR5e and FR3 robots—which lead to task redundancy—and considerable differences in their joint limits, have together resulted in differing workspaces between the two robot mechanisms. As such, the determined target grasp for cloth unfolding would often be unreachable by the robot.

To address this, we developed a simple heuristic pose-correction strategy: when the grasp-detection algorithm provided a grasp pose that could not be reached from the initial position, the textile was repositioned (first closer to, then further from the grasping robot), and a new grasp pose was computed. This approach induced minimal cloth deformation and avoided the need for complex feedback control.

In experimental evaluation over 400 trials across 16 textile items, our heuristic approach increased the number of successful grasp attempts by 6.5 percentage points, raising the attempt rate from 82.5% to 89%. These results show that even basic motion heuristics can effectively mitigate hardware constraints, improving the adaptability and robustness of robotic cloth manipulation systems in real-world applications.

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# Unfolding the challenge: Robotic Solution to Autonomously Unfold Crumpled Garments

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Using robots for tasks involving deformable objects has so far been limited due to constant shape-changing of these objects. This property makes it hard to predict object behaviour as opposed to rigid objects, where shape is constant and thus more deterministic. With the advancement of artificial intelligence, we can develop new technologies in robotics to tackle more sophisticated manipulation challenges. One such challenge is using robots to unfold a crumpled cloth. In 2024, a world-wide robotics competition was organised around this challenge at ICRA (International Conference on Robotics and Automation), designed around a bi-manual robotic cell with UR5e 6-DOF (Degrees of Freedom) robots. We proposed the use of a CeDiRNet-6DOF neural network to unfold cloths crumpled to a random shape. As part of our preparations, we constructed a similar robotic cell with Franka Emika FR3 robots with 7-DOF. A Zed 2i stereo depth camera was used within the cell to asses the state of textile element and its position within the cell. We used this information to estimate the rough shape of textile as part of robotic cell digital twin. This allowed to include textile in collision-avoidance path planning. Additionally, we implemented analytical inverse-kinematics solver for used 7-DOF robots (as opposed to traditionally used numerical solver) to maximise reliability of robot motion. We tested this approach with 16 different textiles and achieved a grasp success of 72.5 % and average unfolding coverage of 58.9 % in our own tests. Compared to 10 other competing state-of-the-art methods [1], we achieved 57 % average coverage on competition set of cloths (8 of 16), which is comparable to the second-best result from the competition. With these advancements as stepping stones, we are making steady progress towards a future where autonomous machines will assist with laundry and other textile tasks.

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# Exploring Electroencephalographic (EEG) Models of Brain Activity using Automated Modelling Techniques

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Electroencephalography (EEG) is a clinical, non-invasive, high-temporal resolution technique for measuring whole-brain activity. However, the underlying mechanisms that give rise to the observed high-level rhythmic activity remain incompletely understood. Various neural population and network models attempt to explain these dynamics, but, to our knowledge, they have not been systematically evaluated.

To explore the space of proposed and potential models, we represent brain networks as graphs, where nodes correspond to brain sources obtained via EEG source analysis. Each node's dynamics are categorized into three subdynamics: synapto-dendritic dynamics (input transformation), intrinsic dynamic, and firing response (output transformation). These subdynamics are defined by a bounded set of functions derived from the literature or generated by an unbounded probabilistic context-free grammar. Such a modular and unbounded specification allows for flexible and physiologically valid construction of the network.

We are currently utilizing our Julia-based framework and are in the model evaluation phase. The dataset we use consists of 64-channel EEG recordings from 50 participants performing a visual flickering task, designed to induce steady-state visual evoked potentials. We repeatedly sample potential EEG models and optimize its parameters using CMA-ES algorithm. Our aim is to determine which established and previously unexamined whole-brain activity models can reproduce the observed oscillations, and, more importantly, which can also accurately capture the harmonics of the stimulation frequency, a robust feature observed in this dataset.

The presence of these harmonic components is a well-documented but not yet fully understood phenomenon in EEG research. By systematically exploring different model configurations, we aim to assess which types of nonlinear models and which features play a crucial role in shaping these spectral patterns. Exploring the set of valid models to understand these mechanisms could have broader implications for theories of whole-brain neural activity and improve our understanding of EEG measurements.

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# Optimization of an energy supply and storage system in residential buildings using a genetic algorithm

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Energy storage plays a crucial role in the transition to sustainable energy systems and local renewable power sources for residential use. Effective storage solutions must be optimized for performance, safety, and efficiency to facilitate widespread adoption. However, identifying the optimal energy supply and storage parameters is a complex challenge due to the multifaceted nature of the issue. This research employs a genetic algorithm (GA) to determine the best configuration for residential energy supply and storage systems, ultimately enhancing their performance and cost-effectiveness.

A computational model was developed to simulate various energy supply and storage scenarios that meet realistic household energy needs. The genetic algorithm was used to optimize key parameters, such as the sizes of photovoltaics, electrolyzers, fuel cells, batteries and hydrogen tanks. The GA works by iteratively evolving a population of possible configurations through processes of selection, crossover, and mutation, allowing it to converge on an optimal solution. The fitness function assesses storage efficiency, safety factors, and economic feasibility based on predefined criteria.

Preliminary findings indicate that GA-driven optimization significantly improves storage overall system efficiency compared to traditional parameter selection methods. The algorithm reveals a trade-off between cost and performance, making combined hydrogen and battery storage a practical option for residential applications. Utilizing genetic algorithms for optimizing the entire energy system represents a promising approach to enhance sustainable energy solutions in homes. By automating the parameter selection process, GA contributes to the development of more efficient and cost-effective storage systems. These findings support broader efforts to integrate hydrogen as an energy storage solution, aiding in decarbonization initiatives and promoting energy self-sufficiency in residential settings.

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# Using Built-in Sensors to Detect Environmental Contact in Collaborative Robots

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Collaborative robots (cobots) are designed to work alongside humans without the need for external safety barriers. However, their limited strength and accuracy, compared to industrial robots, present challenges in precise task execution. Inspired by human strategies for improving precision and handling heavy objects—such as leaning on surfaces for stability or using leverage principles—we investigate how cobots can utilize environmental contact to enhance their performance.

Our research focuses on determining the point of contact without additional external sensors or cameras. Instead, we leverage the robot's built-in sensors, which measure torques in its joints, and apply mathematical models to estimate the contact location from these measured torques. We have developed an approach that successfully identifies the contact point in static conditions and in specific dynamic scenarios in real time, even when the robot's structure is extended and the contact occurs on the extended portion. In Figure 1, the extended structure and the dimensions of the stick are illustrated.

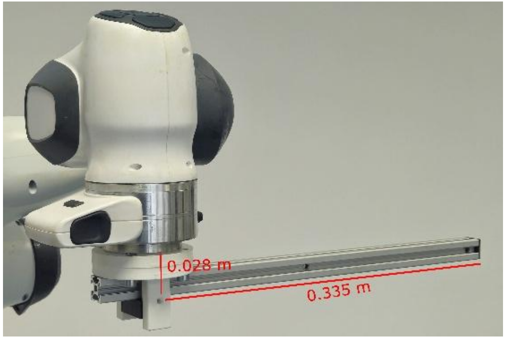

***Figure 2:*** *Robot with a stick mounted on its end effector for extended structure experiments.*

Preliminary results show that our method accurately determines the position of applied forces when the robot is stationary or moving in a controlled manner (i.e., without high accelerations). To achieve this, we formulated a robust estimation model that combines the robot's joint torque data with kinematic parameters in real time.

The next step is to extend this capability to more complex dynamic movements. This research contributes to the broader goal of improving cobot adaptability and precision without relying on additional hardware. By enabling robots to use environmental interactions effectively, we can enhance their utility in various applications, from industrial assembly to human-assistive tasks.

# Nanotechnologies

# 2D Materials and their Application for Supercapacitors

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With increasing industrialization and rapid consumption of fossil fuels, the need for sustainable and renewable energy sources, along with efficient energy storage systems (ESS) has been on the rise. As demand for portable charging devices grows, supercapacitors (SCs) have emerged as promising alternatives to traditional battery systems, offering higher power density, fast charge/discharge cycles and improved efficiency. However, one of the main challenges that SCs face, is energy density, which is influenced by the electrode materials and operating conditions. In this research, we explored the potential of two-dimensional (2D) materials, specifically MXenes, as high-performance electrode materials for SCs. MXenes are a new class of transition metal carbides/nitrides which possess unique characteristics such as high surface area, great electrical conductivity, and abundant active sites. The research focuses on advantages and challenges of using MXenes in SCs, with main focus on the improvement of the SCs energy storage performance by surface functionalization of the MXene using different plasma, as presented in Figure 1. By modifying termination groups on the surface of MXenes, we can improve the capacitance of the material, making them more suitable as electrode materials for SCs applications. In conclusion, while MXenes show great promise in advancing SC technology, further research and development are necessary to address current limitations and fully harness their capabilities for more sustainable and efficient energy storage systems.

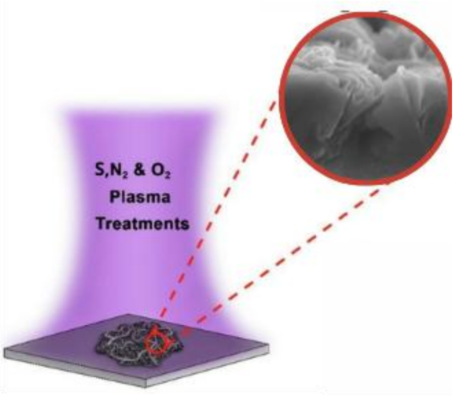

**Figure 1**. Use of different plasma for funtionalisation of MXene powder [1].

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# Numerical Simulations of Pressureless Spark Plasma Sintered (pSPS) Strontium Hexaferrite

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Permanent magnets play an important role in modern devices and enabling technologies as they allow storing, delivering and converting energy. By Volume, Strontium and Barium Ferrites are one of the world's most-used permanent magnetic materials. Although rare-earth magnets exhibit overwhelming superiority in performance the harmful environmental impact of their production, uneven distribution of raw materials and increasingly questionable supply chain force us to look for alternatives. One of the solutions can be found in the group of hexagonal ferrites.

In this study a series of numerical simulations dealing with heat transfer from heating body to the sample via thermal radiation were prepared. Numerical simulations allow us to better describe what happens in a closed crucible. Numerical simulations were prepared from data obtained from a modified SPS apparatus during the sintering process of Strontium hexaferrite in a graphite crucible. The numerical simulations simulated different sample placements in the heating crucible. The results indicate that the position of the sample in the chamber played only a minor role in the differences in the thermal profile of the sample in terms of the maximum temperature difference achieved within the individual sample. As expected, a significant difference in thermal profile evolution occurred for the sample placed in contact with the heating crucible.

**Acknowledgement:** Slovenian Research Agency is acknowledged for funding the research programs (P2-0405, P2-0087-2) and Infrastructure Center for Electronic Microscopy and Microanalysis, Jožef Stefan Institute, Ljubljana, Slovenia (PR-05722).

# Breaking through biofilms: non-specific bacterial targeting with bactericidal nanoblades

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Biofilms present a major challenge in medicine, the food industry, agriculture, and water systems, causing nearly 80% of chronic infections. Their persistence stems from an extracellular polymeric substances (EPS) matrix—a dense network of biomolecules that shields bacteria from antibiotics and disinfectants. In medical settings, biofilms often form on devices like contact lenses, heart valves, and catheters, making infections difficult to treat [1]. Iron oxide nanoparticles (IONPs) offer a promising solution due to their antimicrobial and antibiofilm properties. When functionalized with therapeutic agents, IONPs can be guided by external magnetic fields for targeted biofilm disruption and enhanced drug delivery, improving treatment outcomes [2].

We developed a biofilm removal strategy using functionalized anisotropic magnetic nanoparticles (AMNPs). Under a rotating magnetic field, these nanoparticles generate mechanical forces that break apart biofilms, forming channels that improve antibiotic and disinfectant penetration. We synthesized elongated AMNPs in three sizes—nanochains (<2 µm), nanorods (2–5 µm), and microrods (>5 µm)—through the self-assembly of superparamagnetic iron oxide nanoparticles (~10 nm) [3].

To enhance stability and functionality, we coated these nanostructures with silica and functionalized them with positively charged bactericidal ligands for non-selective biofilm targeting. Characterization was performed using transmission electron microscopy (TEM) and zeta potential measurements, while dynamic light scattering assessed their colloidal stability in different cell media, confirming their suitability for biomedical applications.

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Acknowledgement: This research was funded by the Slovenian Research and Innovation Agency - ARIS: P2-0089, J2-60047, J2-3043, J3-3079, J7-4420, L2-60141, BI-FR/23-24-PROTEUS-005 (PR-12039), BI-RS/23-25-030 (PR-12782).

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# Autogenerated database of High entropy alloys

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High-entropy alloys (HEAs) represent a promising frontier in materials science, yet systematically analysing the vast literature remains challenging.

In this study, we employed Natural Language Processing (NLP) techniques to comprehensively analyse more than 4700 scientific papers, successfully identifying and characterising thousands of distinct HEAs.

Through advanced prompt engineering, experiments with Large Language Models (LLMs), State-Space models (SMM)-Transformer hybrid architecture models, Retrieved-Augmented Generation (RAG) pipelines, we developed a structured database capturing crucial parameters including alloy compositions, phase numbers, and crystallographic structures. Our analysis distinguishes between theoretical and experimental studies, incorporating specific methodological details for each category. For theoretical works, we systematically documented modeling approaches and key computational parameters, while experimental studies are cataloged with their synthesis methods and critical processing conditions.

This database represents the first large-scale, automated extraction of HEA research data. Data accuracy ranges from 90% for HEA synthesis parameters to 97% for HEA composition which outperforms commercially available NLP tools.

| Data | Description | Data Type |
|---|---|---|
| Alloy | Formula of the alloy | String |
| Article Name | Source article title | String |
| Number of phases | N of Crystallographic phases | Integer |
| Experimental or theoretical | Type of details provided | String |
| Experimental details | Details of experiment | String |
| Theoretical details | Theoretical details | String |
| Special conditions | Conditions applied in experiment | String |
| Crystallographic structure | Predicted structure of HEA | String |
| DOI | Source article DOI | String |
| Journal | Published journal | String |

**Table 1.** The schema of the database of the high-entropy alloys.

# Magnetic Attraction Meets Elastic Action: Optimizing Magnetoactive Elastomer Composites

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Magnetoactive elastomers (MAEs) are composite materials consisting of magnetic particles embedded within elastic polymer matrices, allowing their mechanical properties to be tuned in response to external magnetic fields. However, a fundamental understanding of their structure-property-function relationships remains lacking, particularly how processing conditions—such as particle concentration, use of solvent, and magnetic field exposure—affect their magnetorheological behaviour. Most research focuses on exploiting MAE properties rather than optimizing their design through precise material processing. This study aims to bridge this gap, beginning with the incorporation of carbonyl iron powder (CIP) into polydimethylsiloxane (PDMS) matrices. A key focus is to improve filler distribution and matrix interaction through surface functionalization. Our first MAEs were characterized for their rheological and mechanical properties, including stiffness, storage/loss modulus, and damping, under varying magnetic fields. Additionally, anisotropic MAEs will be investigated to enhance magnetic responsiveness while maintaining mechanical flexibility. By establishing key processing-structure-property relationships, this research aims to drive the development of high-performance MAEs for next-generation robotic actuators and adaptive functional materials.

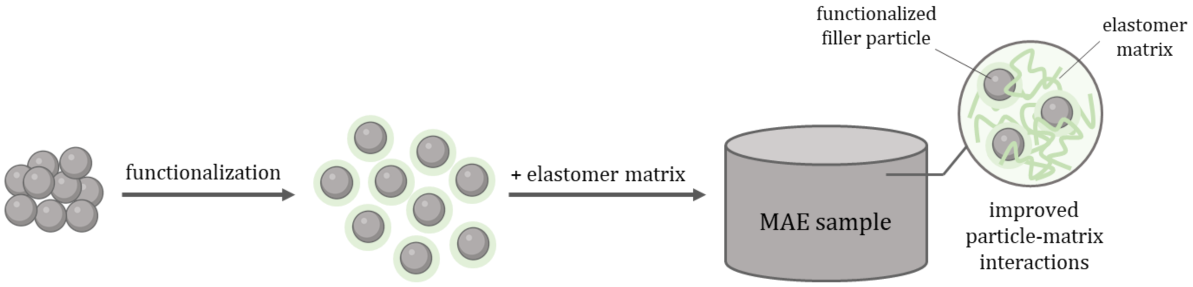

**Figure 1**. Schematic representation of the preparation of MAEs.

Funded by the European Union. Views and opinions expressed are however those of the author(s) 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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# Influence of the functionalization on the chemical stability of barium hexaferrite nanoplatelets

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Nanoparticles (NPs) are particles with at least one dimension below 100 nm. Due to their nano size, they have a high surface-to-volume ratio, making their surface chemistry more highly reactive than that of bulk material. As a result, the physicochemical properties of NPs can be tailored through surface functionalization. In our work, we have been investigating how functionalization affects the chemical stability of barium hexaferrite nanoplatelets (BHF NPLs), a type of nanomagnet. These NPLs were synthesized hydrothermally and subsequently purified using two different methods, with and without an additional acid treatment.

For functionalization, we have used various complexants found in the environment, such as catechols and citric acid. The functionalization was performed in an ultrasonic bath using an aqueous suspension of the NPLs. The chemical stability of the BHF NPLs was analyzed using inductively coupled plasma optical emission spectroscopy (ICP–OES). Our results indicate that complexants accelerate partial dissolution of the treated BHF NPLs initiated by a proton attack.

Acknowledgment

This work was funded by the Slovenian Research and Innovation Agency through the research core funding P2-0089 and research projects, PR-12336 and J2-60038.

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# Exploring the activity of TiON supported ruthenium nanoparticles for the hydrogen evolution reaction

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Hydrogen is a promising alternative to carbon-based fuels in some applications, and water electrolysis is a sustainable method for its production. Consequently, significant research efforts focus on developing highly active and cost-effective catalysts for water electrolysis, where hydrogen evolution reaction (HER) is one of the two half-reactions. In this study, we conducted a computational investigation of TiON- and carbon-supported ruthenium nanoparticles as promising catalysts for HER in alkaline conditions. Experimental observations showed higher activity of TiON-supported catalyst. We explored two possible explanations: (i) metal–support interaction and (ii) the formation of the fcc phase in Ru instead of the thermodynamically stable hcp phase. Our findings suggest that for small nanoparticles, the difference in the stability between fcc and hcp phases is negligible. Similarly, the TiON support does not show a clear preference for any phase, allowing the presence of fcc phase but not favoring it over the hcp one. To assess the effect of TiON support on the activity of nanoparticles, we calculated hydrogen adsorption energies for ruthenium nanoparticles supported on graphene and TiON. The results reveal slightly weaker binding of hydrogen on TiON-supported catalyst, which could facilitate the formation of hydrogen and improve activity towards HER. These insights provide a better understanding of the differences in activity between the two investigated catalysts for HER and may guide the development of superior catalysts.

Acknowledgments:

The authors would like to thank L. Pavko, A. Hrnjić, F. Ruiz-Zepeda, L. Bijelić, and A.R. Kamšek for collaboration.

# DFT-based bonding analysis of thiadiazoles on Cu(111)

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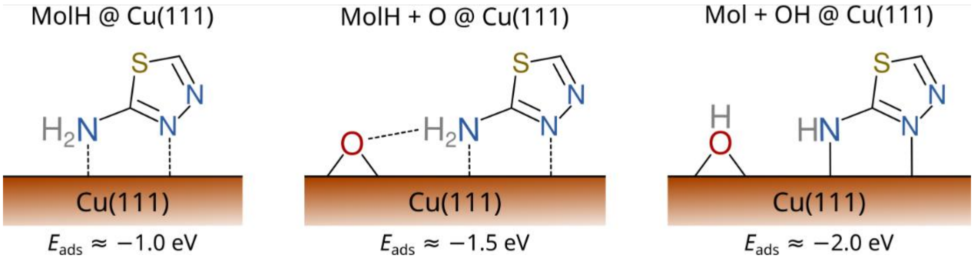

**Figure 1.** Schematic representation of thiadiazole adsorption modes on Cu(111).

Corrosion inhibitors are substances, used in relatively low concentrations, that effectively reduce the rate of corrosion. Among them, unsaturated nitrogen- and sulfur-containing heterocycles, such as azoles, are well-known to inhibit corrosion of copper. In this work, we employed density-functional theory (DFT) to investigate the adsorption of six thiadiazole molecules—a subclass of azoles—on Cu(111), both in the presence and absence of chemisorbed oxygen. Adsorption energy calculations reveal that chemisorbed O atoms enhance molecule–surface binding strength due to several effects. Specifically, oxygen enhances the direct molecule–surface bond by approximately 0.2 eV, enables hydrogen bonding (where possible), contributing an additional 0.3 eV of stabilization, and facilitates X–H (X = N or S) bond cleavage via the $\mathrm{MolH_{(ads)}} + \mathrm{O_{(ads)}} \rightleftharpoons \mathrm{Mol_{(ads)}} + \mathrm{OH_{(ads)}}$ surface reaction, providing about 0.5 eV of additional stabilization. These effects cumulatively enhance the adsorption energy from approximately −1 eV to −2 eV, indicating strong adsorption of thiadiazoles on copper surfaces. Charge-density difference maps reveal clear charge accumulation in the molecule–surface bonding region and around chemisorbed oxygen, confirming the formation of directional chemical bonds. Additionally, projected and integrated local density of states (PDOS and ILDOS) analyses indicate hybridization between molecular orbitals and the Cu surface states, particularly enhanced in the presence of O adatoms. These results provide new evidence that chemisorbed oxygen not only strengthens adsorption but also alters the electronic structure of the adsorbed thiadiazole systems. This is consistent with previous findings for related azole molecules [1–3] and suggests the emergence of a generalizable adsorption pattern across this class of corrosion inhibitors.

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Acknowledgements:

The financial support by the Slovenian Research and Innovation Agency is acknowledged (grants No. P2-0393 and PR-11465).

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# Natural killer cells against glioblastoma: inspecting the battle in a 3D model of glioblastoma

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Glioblastoma (GB) is the most common form of primary brain cancer in adults with poor patient prognosis. The standard of care treatment results in low clinical benefit, indicating an urgent need for novel and efficient therapeutic options. Among these, natural killer (NK) cell-based immunotherapy is a promising approach. NK cells are cells of the innate immune system with an intrinsic capability to recognise and kill cancer cells, including glioblastoma stem cells (GSCs), which play the main role in tumour recurrence. Nevertheless, the anti-GB activity of NK cells may be hampered by the strongly immunosuppressive tumour microenvironment. Understanding of the GB-NK cell crosstalk and various cancer cell resistance mechanisms remains incomplete. To fill this gap, we established and characterised a 3D model of GB and used it as a platform for NK cell-based immunotherapy research. GB spheroids that closely mimic the structure of patients' tumours were prepared from two distinct GB cell types (GSCs or differentiated GB cells) and were co-cultured with NK cells. Ratio-dependent cytotoxicity of NK cells was observed against GSCs and differentiated GB cells. In the spheroid model, cytotoxicity was much higher against the GSCs compared to the differentiated GB cells, even though NK cells more efficiently infiltrated spheroids of differentiated GB cells. This was consistent with the analyses of cytokine secretion, which indicated that higher concentrations of immune cell chemoattractants were released from differentiated GB cells compared to GSCs. Our results shed light on the important factors in the GB-NK cell crosstalk that may regulate NK cell activity and the immune landscape of the GB microenvironment.

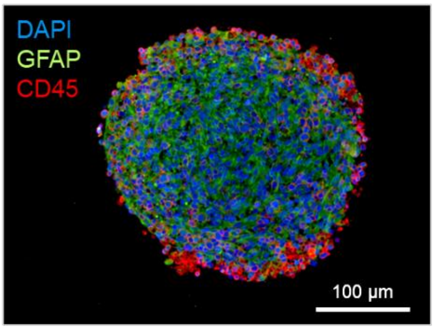

**Figure 1**. Immunofluorescent staining of GB spheroid (green) cocultured with NK cells (red). Cell nuclei are stained in blue.

# Copper chloride–N-alkyl triethylenediamine compounds in composition space diagram

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The **copper chloride – HCl - voluminous organic polyamine composition diagrams** were discovered in the present study. Earlier published articles, which describe the synthesis and characterization of **N-alkyl triethylenediamine chlorocuprates**, do not cover all possible coordination compounds potentially present in such systems[1], [2], [3], [4]. However, some of these compounds are known for their catalytic, piezoelectric and photoelectric properties[4]. These factors were the reason: 1) for the systematic investigation of these systems based on the use of two-dimensional composition diagrams; 2) for studying their chemical and physical properties.

**Solvothermal syntheses** were carried out at 150 °C for 5 days, CuCl or mixture of copper powder and $CuCl_2$, HCl, and triethylenediamine (1,4-diazabicyclo[2.2.2]octane or DABCO) as starting reagents, and ethanol or methanol as solvents and starting reagents simultaneously. After cooling down to the room temperature, the crystals of **$[N, N'\text{-}Et_2DABCO^{2+}]_2[Cu_3Cl_7]^{4-}[H_2O]$** (space group $I4_1/a$, Z=16, **inorganic part–** isolated $Cu_3Cl_7$ cluster), **$[N, N'\text{-}Et_2DABCO^{2+}][CuCl_3]^{2-}[H_2O]$** (space group $P4_32_12$, Z=8, isolated inorganic dimer $Cu_2Cl_6$), **$[N, N'\text{-}Et_2DABCO^{2+}][CuCl_4]^{2-}$** (space group $P2_12_12_1$, Z=4, isolated $CuCl_4^{2-}$ tetrahedra), **$[N\text{-}Et, N'\text{-} MetDABCO^{2+}][CuCl_4]^{2-}[H_2O]$** (space group Cc, Z=4, isolated $CuCl_4^{2-}$ distorted tetrahedra), **$[N, N'\text{-}Met_2DABCO^{2+}]_3[Cu_2Cl_4]^{2-}_3$** (space group $P2_1/n$, Z=4, $[(Cu_2Cl_4)^{2-}]_n$ infinite chains), **$[(N\text{-}MetDABCO^{+})_2\ Cu_4Cl_6][CH_3OH]$** (space group $P2_12_12_1$, Z=4, isolated cluster $Cu_4Cl_6^{2-}$ coordinates 2 polyamine ligands), **$(N\text{-}MetDABCO^{+})CuCl_3(H_2O)$** (space group R3, Z=3, isolated $CuCl_3(H_2O)^{-}$ cluster coordinates 1 polyamine ligand) appeared at the bottom of the Teflon lines. The obtained compounds were characterized by **single-crystal X-ray diffraction** and **Raman spectroscopy**. Also, **the catalytic properties** of these compounds were studied in the reaction of cyclohexane to cyclohexanol oxidation by hydrogen peroxide. In conclusion, the physical and chemical properties of compounds require deeper investigation.

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# Corrosion of 3D printed aluminium alloy AlSi10Mg

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Corrosion is a spontaneous process of material degradation that affects metals. With advances in modern technology, a new production method of additive technology has been presented in the world of metallurgy. With this technique, the desired object is built by stacking thin layers one atop another. It enables the production of complex internal structures and quick production of prototypes. While the waste material of the manufacturing process is reduced, we are also presented with a unique microstructure that is quite different than when manufactured by traditional casting or annealing. In the case of additive manufacturing (3D printing), the microstructure elements resemble cast microstructure (Figure 1) but with finer components (due to high local temperatures and fast cooling gradients). Due to higher energy levels on grain boundaries and defects, microstructural elements and their size play an important role in material degradation. These high-energy areas are more likely to become initial spots for corrosion. Another important parameter in corrosion resistance properties is the change in chemical composition, which is required to accommodate specific manufacturing requirements of the material. Much like grain boundaries and defects, different electrochemical potentials of microstructural elements represent initiation areas for corrosion.

This study focuses on effects of chemical composition and microstructure change on corrosion properties of wrought aluminium alloy 4004 (in cast state), cast aluminium alloy Silafont36 (AlSi10MgMn alloy, widely used for casting, cast state) and aluminium alloy AlSi10Mg for 3D printing (AlSi10Mg alloy with minimal amount of impurities, in 3D printed state). In addition, the formation and efficiency of zirconium-based conversion coatings will be examined. Since conversion coatings start forming around the defects in the material, it is expected for conversion coatings to vary regarding the production method of the substrate material.

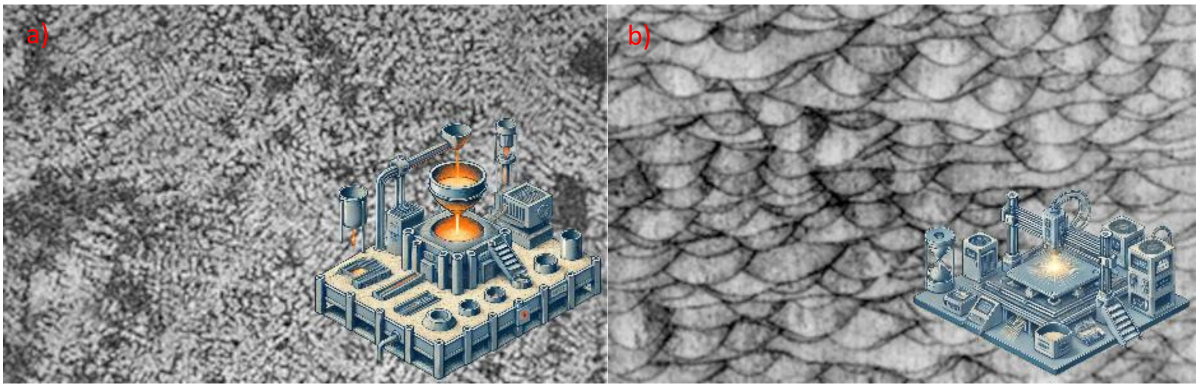

**Figure 1**: a) Cast and b) 3D printed aluminium alloy microstructure.

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Acknowledgements: The financial support by the Slovenian Research and Innovation Agency is acknowledged (grants No. P2-0393 and PR-12845).

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# Fluorinated Siloxane-Silica Hybrid Sol-Gel Coatings for Long-Term Corrosion Protection of AA2024-T3

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Aluminium alloy (AA)2024-T3 is composed of aluminium (~94.7 wt. %) and other alloying elements such as copper (~4.5 wt. %), magnesium (~1.5 wt. %), manganese (~0.6 wt. %), and iron (~0.2 wt. %). It is widely used in the aerospace industry due to its appropriate mechanical properties but is prone to corrosion in chloride-rich environments due to its alloying elements [1]. Although chromium(VI) --based coatings offer excellent protective properties, their use in many countries is restricted due to their negative impact on the environment and human health. One often-studied alternative is sol-gel coatings, which are efficient barrier protection on alloy surfaces [2], [3]. This study aimed to synthesize the coating using fluorinated siloxane-silica sol-gel systems to enhance the corrosion resistance of the underlying AA2024-T3 metal substrate. The coating was prepared from the inorganic precursor tetraethyl orthosilicate and organic precursors methyl methacrylate, 3-(trimethoxysilyl)propyl methacrylate, and a small amount of 2,2,2-trifluoroethyl methacrylate. The characterization was performed using real-time Fourier transform infrared spectroscopy to monitor the chemical reactions during preparation. Surface characterization of fluorinated siloxane-silica coatings deposited on AA2024-T3 substrates was conducted using field emission scanning electron microscopy combined with energy-dispersive spectroscopy to evaluate surface morphology and elemental composition. Corrosion properties were monitored in a 0.1 M NaCl solution using electrochemical impedance spectroscopy over an extended immersion period. The results confirmed that the synthesized coating offered improved corrosion protection, with 2,2,2-trifluoromethyl methacrylate enhancing barrier properties and maintaining stable impedance over extended immersion, outperforming previous studies [2], [3].

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# Oxide thin film as a protection of photocathode from photocorrosion in water splitting

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The production of green hydrogen as a fuel is becoming more and more important due to global warming and energy crisis. We focused on hydrogen production, where the energy needed for water splitting is harvested from solar light. The photocathode, where the hydrogen evolution reaction occurs, is composed of oxide material grown on semiconductor, immersed in aqueous environment[1], [2], as presented in Figure 1. To protect semiconductor from harsh electrolytic environment, thin oxide film is used on the semiconductor to prevent photocorrosion of semiconductor. Therefore, we produced a photocathode based on strontium titanate ($SrTiO_3$, STO) grown epitaxially on germanium substrate using pulsed laser deposition (PLD). Crucial step for obtaining epitaxial growth of STO was the deposition of STO seed layer, resulting also in atomically sharp interface. Photoelectrochemical (PEC) measurements were performed on oxide protected and non-protected photocathode, where measurements of STO on Ge showed higher currents at lower onset potential compared to bare germanium. Surface morphology was investigated with scanning electron microscope, where we observed significant damage of bare germanium surface after PEC (Figure 2) compared to the one protected with STO.

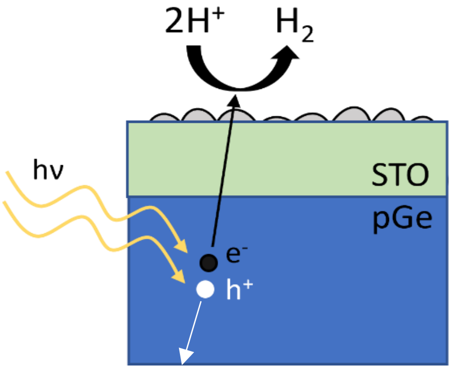

**Figure 1**. Photocathode structure and working principle

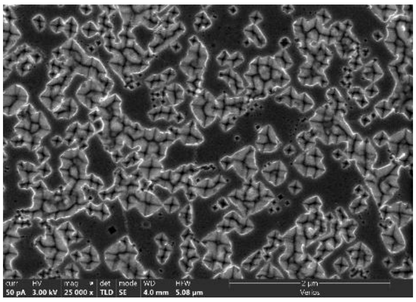

**Figure 2**. Damaged germanium surface due to photocorrosion

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# Metrological approaches for biofilm identification on solar panels

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Harvesting energy from the sun is a crucial renewable technology. Solar panels have also become a new environment for organisms to conquer, including a seldom investigated group of extremophilic fungi. The formation of biofilms on solar panels significantly decreases electricity production yet remains largely unexplored.

In our research project, we aim to design and implement nucleic acid-based quantification methods to rapidly identify the solar panel biofilm communities (Figure 1). These methods, along with appropriate reference materials, will adhere to core metrological principles to ensure accuracy, precision, repeatability, and traceability.

Thus far, we have obtained samples from a solar panel facility in Ljubljana, which we used to identify the core biofilm-forming fungal species through two approaches: mass spectroscopy of protein profiles and DNA barcoding. We selected four of the most abundant fungi as model organisms, proliferated them on agar plates, lyophilized them, and extracted the total genomic DNA. This DNA was used for whole-genome sequencing and to prepare reference materials for quantification. Two commercially available DNA extraction kits were evaluated for yield, purity, and fragmentation to identify the most suitable protocol.

In the final phase of the project, we will design novel, organism-specific digital PCR (dPCR) assays to detect and quantify the selected fungi. These novel assays could form the basis for biofilm monitoring and aid stakeholders in developing novel strategies for biofilm mitigation that would improve the efficiency of solar panels.

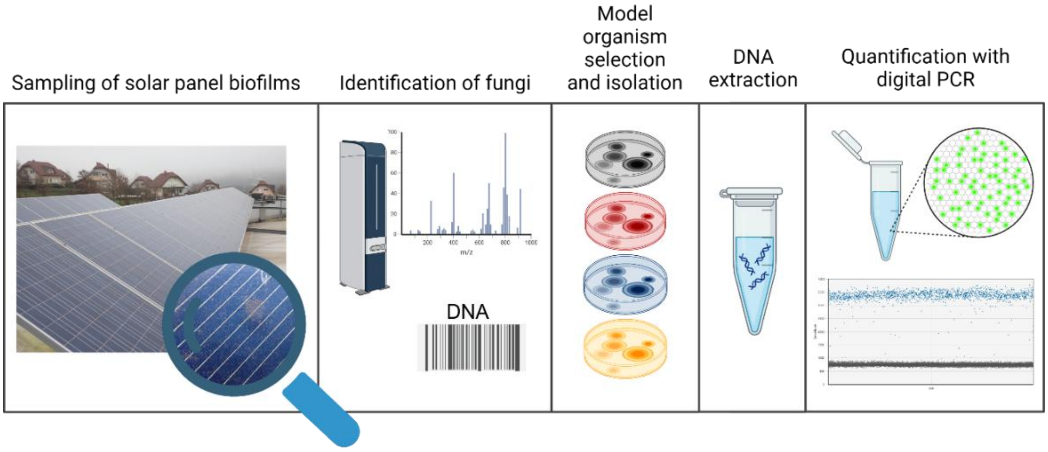

**Figure 1**. Graphical abstract. Created in BioRender.com

# Using Honey Bees and Their Products to asses Environmental Pollution by HRMS-based Techniques

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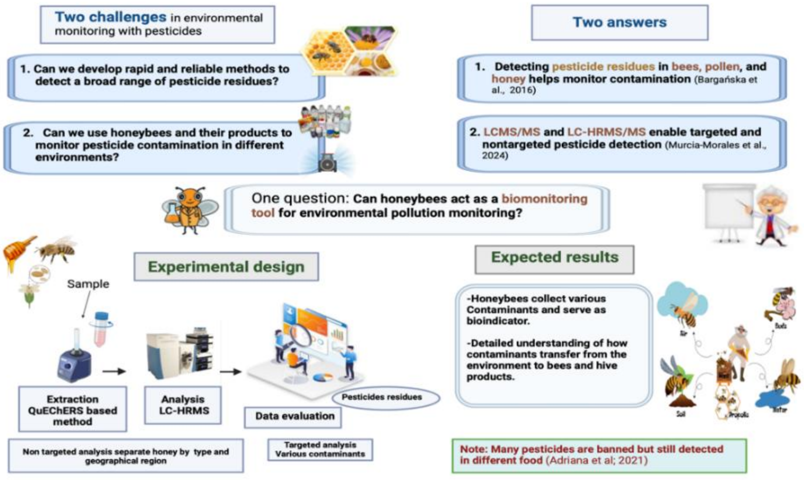

Nowadays chemicals called pesticides are frequently employed in agriculture to eradicate weeds, insects, and other pests, and due to their persistence and nonselective toxicity they contribute to environmental pollution. Honeybees and their products (pollen, honey, and wax) serve as biomonitors of environmental contamination by toxic substances, which offer important details about environmental pollution. Two challenges are arising, the first one is related to the development of rapid and reliable methods to detect a broad range of pesticide residues, and the second one on the effectiveness of using honeybees and their products to monitor pesticide contamination in different environments. To this end, my research aims to develop and verify a quick, accurate, and reliable approach for qualitative and quantitative determination of pesticide residues from several chemical classes in honey bees and their products. Bee, pollen and honey samples have been collected from grassland, urban areas, and agricultural landscapes of Slovenia and multiple honey samples will be obtained from France. I propose to use QuEChERS (quick, easy, cheap, effective, rugged and safe) method, coupled with solid-phase extraction cleanup to extract the pesticide residues from the samples. The samples will then be analyzed using LC-MS/MS (Liquid chromatography tandem-mass spectrometry) to quantify preselected pesticides. For the identification of unknown or suspect contaminants the LC coupled to high-resolution mass spectrometry (HRMS) analysis will be used. We expect that this study will uncover various pesticides and other organic contaminant residues in honeybees and their products and demonstrate that honeybees can serve as biomonitors of environmental pollution. Finally, the study in its wider frame tests the hypothesis stress response of honeybees in relation to the environmental pollution with organic chemicals, which contributes to the projects WellBEEing and PARC 4.3 studies on innovative approaches connecting environment and food.

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# Allele-Specific Expression Analysis in Tetraploid Potato Reveals Stress-Induced Transcript Switching Under Heat Conditions

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Plant genomes often exhibit high ploidy and repetitive content, presenting significant challenges for expression analysis of highly similar transcripts, particularly when using short-read RNA-seq approaches. To address these limitations, we developed a computational pipeline that uses long-read RNA-seq data to analyze allele-specific expression in tetraploid potatoes under heat stress conditions. Long-read RNA-seq technology enabled us to resolve highly similar transcripts and perform detailed allele-specific expression analysis, providing insights into regulatory mechanisms activated during stress response. Our analysis identified genes that undergo major allele expression switching under heat stress, revealing potential adaptive mechanisms. These findings enhance our understanding of polyploid gene regulation under environmental stress and offer valuable resources for crop improvement strategies targeting heat tolerance in potato and related polyploid crops.

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# Novel Polyethylene Glycol Acrylate - Based Ceramic Slurries for Digital Light Processing

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Additive manufacturing of ceramics has steadily gained popularity and recognition over the past decade as one of the rare methods capable of producing spatially complex ceramic structures. Among the various techniques, Vat Photopolymerization (VPP) represents one of the most popular family of techniques, all relying on the same fundamental principle: the use of ceramic particle suspensions in photo-polymerizable organic media - commonly known as ceramic slurries.

Ceramic slurries of high quality, although expensive, are available commercially. However, the selection of ceramic materials remains limited, and the exact formulations are a trade secret, known only to the manufacturer. Since such slurries are already highly loaded with solid particles, their physical properties are very sensitive to even minor compositional changes, making any modifications difficult. For these reasons, the development of ceramic slurries is an important topic within the VPP research community, still facing many challenges.

In this presentation, we introduce a novel, highly loaded (80 wt%) aluminium oxide ceramic slurry based on a polyethylene glycol acrylate system, specifically designed for processing on the CeraFab S65 Digital Light Processing (DLP) platform. This formulation offers adjustable rheological profiles and excellent photo-curing rates under 460 nm blue light.

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# Modeling the earliest stage of aluminum oxidation with kinetic Monte Carlo

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Developing accurate and predictive models of complex processes that take place over long time and length scales is at the forefront of materials science research. To model such processes, one often has to sacrifice accuracy for computational efficiency. One method—that allows for highly accurate simulations even at the mesoscopic scale and has been particularly successful in simulating processes relevant for heterogeneous catalysis—is known as kinetic Monte Carlo (kMC) [1]. We aim to develop a general computational framework for performing such simulations. Here, the first steps toward this goal will be presented, focusing on simulating oxygen adatom diffusion on the aluminum surface during the earliest stage of aluminum oxidation (Figure 1). Through an on-lattice kMC simulation—performed with the novel framework—we study the formation and morphology of oxygen islands, which are known to form when oxygen coverage is still below one monolayer. Our findings are compared to experimental data available in the literature as well as previous similar simulations [2]. This study serves as a stepping stone on the way to simulating the process of aluminum oxidation, which in turn should serve as a prototypical model of how to simulate such complex processes.

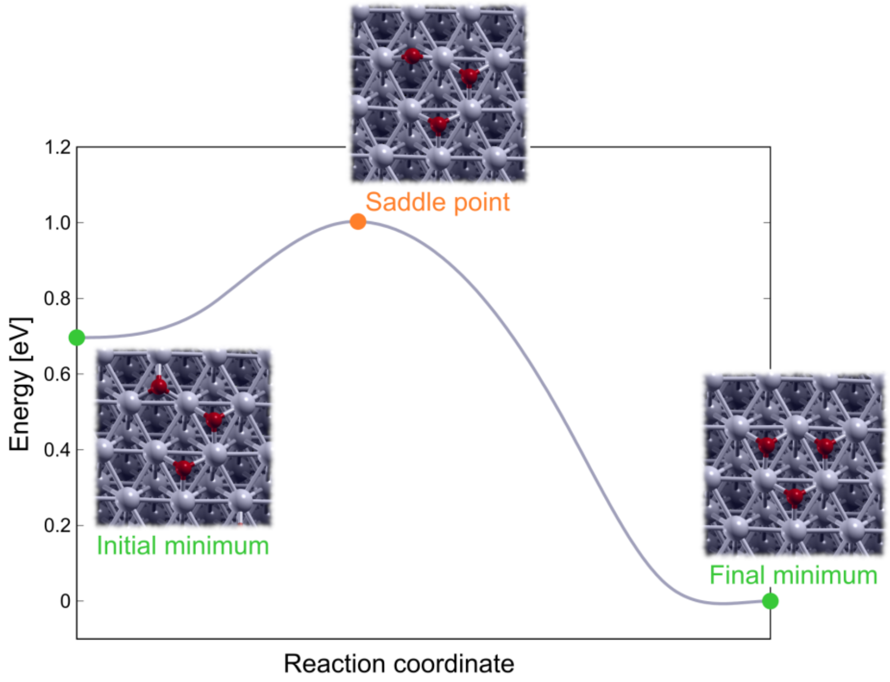

**Figure 1**. Energy diagram of the formation of a three adatom oxygen island.

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# Development of a Low-Cost Ionic Wind Propulsion System

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Electrohydrodynamic propulsion using ionic wind thrusters offers a promising route for compact propulsion systems. However, existing designs are often complex or costly. This research aims to develop a low-cost, easily assembled air ionic wind plasma thruster for atmospheric-pressure applications.

The thruster was constructed using 3D-printed supports and copper-tape electrodes, with an off-the-shelf high-voltage transformer to ionize ambient air and generate an electric wind. Wind speed was measured with an anemometer at varying distances from the outlet. Experiments were conducted under different electrode polarities and with a two-stage electrode configuration to optimize thrust generation.

Measurements revealed a near-linear decrease in wind speed with increasing distance from the thruster exit. Operation under negative polarity produced roughly 10% higher wind speeds compared to positive polarity. The two-stage configuration enhanced thrust by approximately 20% relative to a single-stage setup. While a protective acrylic tube reduced performance by about 15%, it significantly improved safety. Prolonged operation with the small high-voltage transformer resulted in thermal overload, diminishing output performance.

The results validate the thruster design as a viable, cost-effective platform for studying atmospheric-pressure plasma and electrohydrodynamic propulsion. The device's simplicity and modular design make it suitable for both research and demonstration purposes, with further potential for optimization in electrode geometry and power delivery.

# Hydrothermal transformation of Aurivillius $Bi_4Ti_3O_{12}$ platelets into two-dimensional $ATiO_3$ (A=Sr,Ba,Ca) perovskites: Mechanisms and Prospects

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Topochemical conversions (TC) of layer-structured Aurivillius phase $Bi_4Ti_3O_{12}$ platelets into $ATiO_3$ (A = Sr, Ba, Ca) perovskites have been intensively studied in molten salts (NaCl/KCl) at 660 °C-1100 °C. A more intriguing approach has recently been achieved at much lower temperatures (~ 200 °C) using the hydrothermal method. Nevertheless, the mechanistic control of reaction pathways and the product properties remain underexplored. The TC of $Bi_4Ti_3O_{12}$ to structurally similar $SrTiO_3$ (lattice mismatch ~2%) was confirmed to proceed through the dissolution of $Bi_4Ti_3O_{12}$ and the $SrTiO_3$ epitaxial growth over the template basal surface planes, leading to formation of $SrTiO_3/Bi_4Ti_3O_{12}$ heterostructures at the intermediate stage and $SrTiO_3$ platelets upon complete transformation (Figure 1) [1]. On the contrary, the higher structural mismatch between $Bi_4Ti_3O_{12}$ and $BaTiO_3$ (4%) does not allow preservation of two-dimensional (2D) shape under the same conditions. However, other recent studies reported in-situ hydrothermal transformation of $Bi_4Ti_3O_{12}$ into $BaTiO_3$ with a maintained 2D shape by means of a small amount of sodium oleate, which presumably regulates the dissolution of specific structural units in the Aurivillius phase (Figure 1) [2]. However, the exact transformation mechanism remains unclear. Such well-defined 2D $ATiO_3$ perovskites with exposed (100) facets have great potential in various fields, including piezoelectrics, piezocatalysis, and photocatalysis/catalysis.

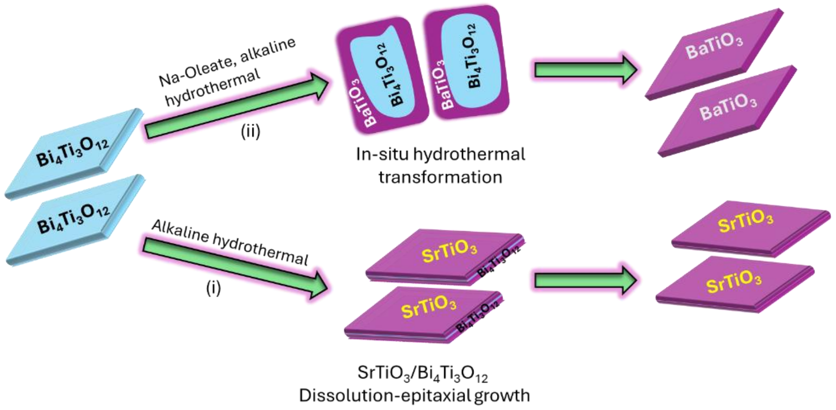

**Figure 1.** Schematic presentation of the $Bi_4Ti_3O_{12}$-to-$ATiO_3$ hydrothermal transformation: (i) dissolution-epitaxial growth and (ii) *in-situ* transformation.

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# A Novel Polymorph of $VOF_3$: Structural Characterisation and Synthesis

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Polymorphism is a phenomenon where the same compound crystallizes in different crystal structures. The investigation of polymorphism is important because variations in crystal structure can lead to different physical and chemical properties [1].

Vanadium(V) trifluorideoxide, $VOF_3$, is notable for its applications in the oxidative coupling of phenols in organic synthesis [2]. It is also a Lewis acid and forms neutral complexes with oxygen- and nitrogen-donor ligands [3] and diverse fluoridooxidovanadate(V) anions with fluoride-ion donors [4]. The crystal structure of $VOF_3$ was first reported over 50 years ago and later redetermined [5,6]. We identified a novel polymorph and characterised it by single-crystal and powder X-ray diffraction, as well as by Raman spectroscopy. The crystal structure of a new polymorph exhibits a cube-like octameric unit interconnected into a double layer, whereas the previously reported polymorph adopts a corrugated layer structure built from edge-sharing dimers (Figure 1). The interconversion between these polymorphs was studied.

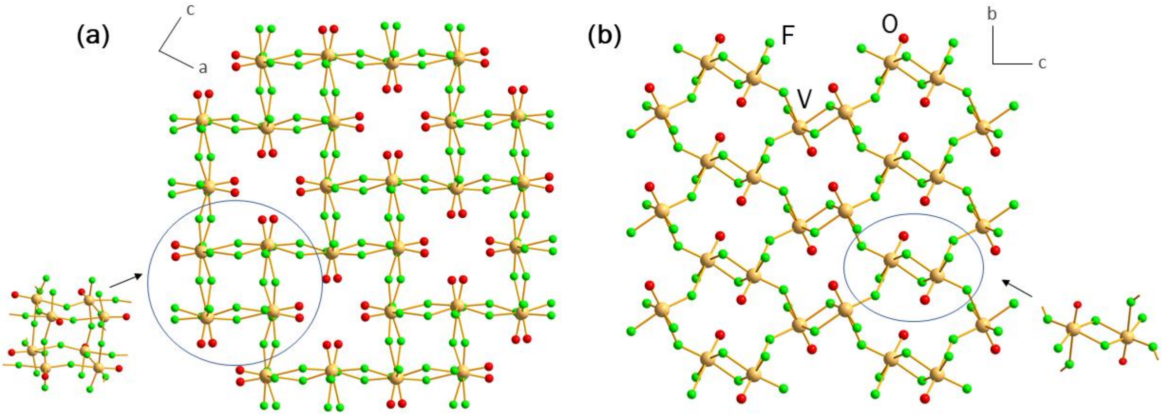

**Figure 1**. a) Double-layered structure of the new $VOF_3$ polymorph and b) the corrugated layer observed in the previously reported $VOF_3$ polymorph,

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# Optimizing Spark Plasma Sintering Conditions for Texture Retention and Enhanced Magnetic Properties of Bulk Nanocrystalline Nd-Fe-B Magnets

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The transition to green technologies, namely electric vehicles and generators, requires the development of cost-effective and sustainable high-performance hard magnetic materials. Among these, rare-earth transition-metal (RE-TM) Nd-Fe-B-type magnets based on the $Nd_2Fe_{14}B$ hard-magnetic phase exhibit the highest maximum energy products $(BH)_{max}$ up to 474 kJ/m$^3$, making them the most promising candidates for energy-conversion applications [1]. Crystallographic alignment of hard-magnetic grains along their c-axis (easy direction) maximizes the remanence (Br) and improves the energy product which scales quadratically with Br. Enhancing the $(BH)_{max}$ and remanence through texturing is therefore a key strategy for optimizing magnetic performance.

The Hydrogenation-Disproportionation-Desorption-Recombination (HDDR) process is widely used to produce fine-grained, anisotropic magnetic powders [2]. Their submicron grain size reduces the need for costly coercivity-enhancing Heavy rare earth (Dy, Tb). A hot-pressing Spark Plasma Sintering (SPS) technique was utilized to consolidate HDDR-type $Nd_{28.24}Fe_{70.70}B_{1.06}$ (wt.%) powder under rapid densification to limit grain growth. This study examines how varying SPS pressure (12–64 MPa) affects remanence and $(BH)_{max}$. Ram displacement (mm), reflecting shrinkage and thermal expansion was monitored to determine the lowest sintering temperature for a given pressure, mentioned in Figure 1. A constant 50 °C/min heating rate was applied. As shown in Table 1, lowering the pressure from 64 to 12 MPa raised the sintering temperature from (722 - 858) °C to achieve full density. All samples reached near-complete densification with minimal grain growth and similar coercivity (Hci) values of 1007-1021 kA/m. The highest (BH)max of 207 kJ/m$^3$ was achieved at 25 MPa, suggesting moderate pressure best preserves texture. Further work is needed to elucidate relations between the applied pressure and final texture.

**Table 1.** SPS conditions and magnetic properties.

| Pressure MPa | Densification T (°C) | Br [T] | Hci [kA/m] | (BH)max [kJ/$m^3$] | Density [g/$cm^3$] |
|---|---|---|---|---|---|
| 64 | 722 | 1.068 | 1007 | 197 | 7.59 |
| 51 | 735 | 1.014 | 1037 | 180 | 7.55 |
| 38 | 765 | 1.021 | 1029 | 183 | 7.51 |
| 25 | 808 | 1.089 | 1022 | 207 | 7.54 |
| 12 | 858 | 1.059 | 1021 | 198 | 7.51 |

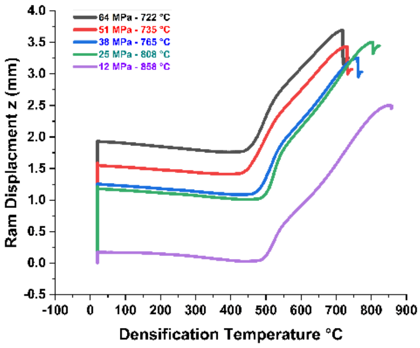

**Figure 3.** Ram displacement with respect to densification temperatures.

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# A novel PIMD method for the simulation of spin-phonon coupled systems

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The research of new materials represents a huge area of interest at the moment, magnetic materials in particular. To understand these systems better and improve the search algorithms, it is important to be able to simulate them accurately and efficiently. We developed a new method based on Path Integral Molecular Dynamics (PIMD) which can simultaneously treat both the electronic and the vibrational part of the problem, and which is capable of overcoming the limitations of the state-of-the-art monte carlo approaches. We have explored the low temperature behaviour of antiferromagnetic materials capable of undergoing a spin-Peierls phase transitions and explained how the spin-spin correlation changes upon the inclusion of the spin-phonon coupling, as well as the importance of quantum-machanical description compared to classical description when simulating such systems. Understanding the spin-spin correlation tells us how the locality of the information is affected upon phase transition, and how applicable such a method could be at simulating and finding materials which exhibit such phase behaviour much faster than it would be to actually synthesise it and test its properties. We hope that in the future we can extend the method and search for new realistic materials in a faster and more accurate way.

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# Functionalized Erythrocyte Vesicles for Targeted Breast Cancer Therapy

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Among Neuropeptide Y receptors (NPYR) -positive breast cancers, Y1R is detected in 100% of tumor samples but only in 58% of normal breast tissue, making it a promising target for selective drug delivery [1]. Erythrocyte membrane vesicles (EMVs) offer a biocompatible and stable nanocarrier system with immune evasion and prolonged circulation, providing a potential strategy for receptor-targeted therapy [2]. This study investigates the development and characterization of NPY-functionalized EMVs for targeted breast cancer therapy.

EMVs were generated from human erythrocytes via hypotonic lysis, followed by sonication and extrusion to create stable nanoscale vesicles. Western blot analysis confirmed the retention of key erythrocyte membrane proteins (CD47, CD35, Band 3) throughout processing. Proteomics with in-gel fractionation and proteolytic digestion assessed the protein composition. Samples were separated on SDS-PAGE precast gels, cut into four fractions per lane, digested with trypsin, and analyzed using nano LC-MS/MS. For functionalization, NPY analogs were conjugated to EMVs via maleimide-thiol chemistry. SDS-PAGE confirmed successful conjugation, while ongoing efforts focus on optimizing purification and characterization. Characterization included dynamic light scattering for size, zeta potential for surface charge, and transmission electron microscopy for morphology assessment.

Preliminary findings confirm the retention of key membrane proteins and successful NPY conjugation, with further investigations underway to evaluate vesicle stability, surface charge, and receptor targeting efficiency. This study applies the foundation for biomimetic vesicle-based drug delivery into clinical applications, advancing precision oncology and targeted therapeutics for breast cancer patients, bridging the gap from research to reality.

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# Preparation of magnetic Janus nanoplatelets

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Janus particles are symmetric particles with asymmetric surface properties. Since Paul deGennes introduced the term Janus particles three decades ago, their unique surface properties have made them a subject of extensive research with promising applications [1]. Our study aims to functionalise one face of permanently magnetic barium hexaferrite (BHF) nanoplatelets (NPLs) with polar ligands. By dispersing so-prepared nanoplatelets in nonpolar solvents we seek to develop the first magneto-electric liquid. Since the magnetic properties of such material can be altered with the electric field and vice versa, magneto-electric liquids are intriguing materials for sensors, actuators etc.

To prepare Janus particles via surface modification, only one face of the NPLs must be functionalised. In our study, we protected one face of the NPLs by their immobilization on the glass substrate. The deposition was performed in a magnetic field, to ensure uniform orientation, exposing the same face of the NPLs for subsequent functionalization with polar organic ligands. Lastly, the particles were harvested from the glass substrate and dispersed in water. The quality of the deposition of the NPLs on the substrate and subsequent harvesting were determined with a scanning electron microscope.

Upon the addition of hexanol to a suspension of harvested NPLs, the Janus NPLs assembled at the water–hexanol interface. This behaviour points to the asymmetric, Janus character of the NPLs, since the polar ligands on the functionalised face of the platelets are solvated by hexanol but insoluble in water, thus favouring hexanol, while the untreated, hydrophilic face remains in water.

In the future, these findings will provide a crucial foundation for the development of novel liquid magneto-electric materials, paving the way for advancement in sensing and other technologies.

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## Acknowledgment

The study was funded by the Slovenia Research and Innovation Agency through the research core funding P2-0089 and P1-0192, and the research project PR-12851. The study was also partly funded from the European Union's Horizon 2020 research and innovation programme by the project MAGNELIQ 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.

# Elucidating mysteries from the CuBr – HBr – DABCO system

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Coordination compounds of copper(I) halides and organic polyamine ligands are often described as candidates for new catalysts in various organic reactions and as replacements for inorganic materials containing rare-earth elements used as phosphors in LEDs [1], [2]. Before our research began, only five compounds were known from the ternary system CuBr – HBr – DABCO. Through a systematic investigation of the chosen ternary system using solvothermal and electrochemical synthesis, we successfully prepared and determined the crystal structures of six new compounds from this system. During abstract preparation, some of our products were tested for photoluminescent properties, and preliminary tests showed some promising results (Figure 1). The structures of the obtained compounds, along with the photoluminescent measurement results, will be presented at the conference.

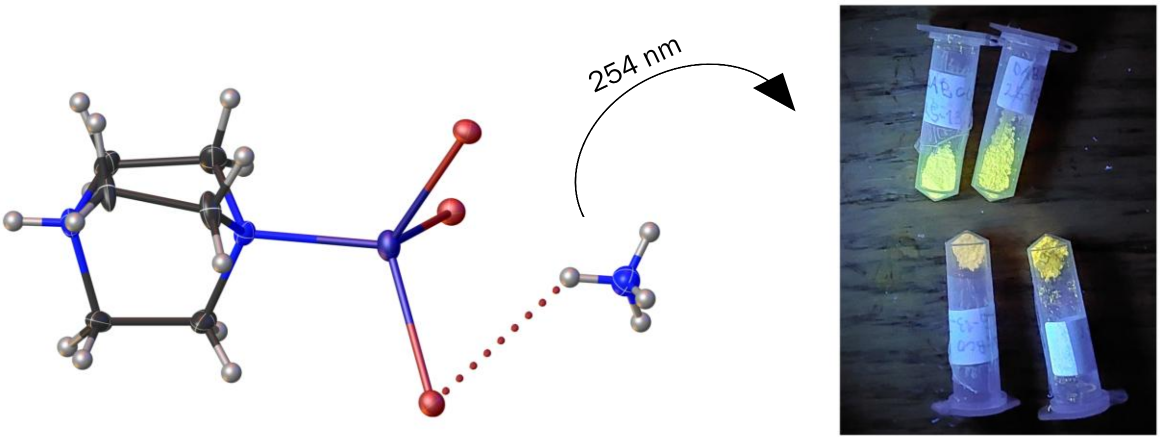

**Figure 1**. Structure of the [H*dabco*]CuBr$_3$NH$_4$ product shows some luminescence under 254 nm UV light.

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# Atomistic modeling of cobalt boride as catalysis materials for water electrolysis

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Transition-metal Co-based X-ides (X = B, P, S) have been experimentally identified as promising catalysts for direct seawater electrolysis [1]. In this study, we investigate two CoB-based materials that have been experimentally synthesized. The first material consists of fcc-structured Co nanoparticles doped with a small amount of boron (0.5 at%), whereas the second material is $Co_2B$, which has a tetragonal crystal structure. To understand why only a tiny amount of B can be doped into Co experimentally, we performed density-functional theory (DFT) calculations for both materials. The results indicate that doping Co with boron is endothermic by about 0.2 eV per B atom, explaining why experimentalists succeeded in incorporating only a small amount of B into Co. Despite this endothermicity, calculations reveal that B atoms prefer to segregate to the Co bulk, i.e., a B atom is 0.3 eV and 0.2 eV more stable in the fcc-Co bulk octahedral interstitial site than in the surface hcp-hollow site and the subsurface octahedral interstitial site, respectively.[1] In contrast, for $Co_2B$, the calculated formation enthalpy is exothermic, with a value of approximately −0.8 eV per $Co_2B$ formula unit.

As a side note, it is worth mentioning that boron itself is an amazingly interesting element [2]: it is extremely hard and possesses a surprisingly complicated crystal structure consisting of 111 atoms in a rhombohedral unit cell [3]. It also has a remarkably high melting point of 2349 K.

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[1] This result contradicts the experimental observation that the amount of B is enriched at the surface. However, this surface enrichment may be due to surface oxidation.

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# Fractional topological charges in 2D nematic liquid crystal

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In this study, we investigate the fractional topological charges in two-dimensional (2D) nematic liquid crystals (LCs). Using the Landau–de Gennes phenomenological model, we describe the nematic LC order in terms of the tensor order parameter and its associated free energy, formulated using tensor invariants. Through mathematical modelling and simulations, we analyze geometrically imposed fractional charge and their manipulation by time variation of appropriate external electric fields. In particular, we illustrate that via sharp confining boundaries one could stabilize any fractional charge. Furthermore, the latter could by changed only by discred values due to the inversion symmetry of the nematic LCs.

# Sensor technologies

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# Electrochemical sensor for detection of benzotriazole in water

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Persistent mobile chemicals (PMCs) are the result of the development of modern organic chemistry, which has been found nowadays in tens of thousands of everyday products. Although PMCs have been around for many years its negative effects on human health are only beginning to be understood.[1] Our aim is to create new types of electrochemical sensors customised for PMC detection in on-site environments. Data from new sensors will help build and refine assignment and pathway models, enabling an effective and efficient reduction of PMCs in the environment.

In the present work we will discuss the development of receptor element for detection of benzotriazole (BTA). BTA is extensively utilized in various industries for its properties as corrosion inhibitor, UV radiation filter, and plastic stabilizer. BTA is, therefore, found in food packaging, dishwashing detergents, textiles, lubricants, antifreeze, aircraft de-icing fluids, and other commercial and industrial products.[2] Currently, the primary methods for analysing BTA in environmental samples involve solid-phase extraction followed by GC-MS or LC-MS. However, there is a need for cost-effective, fast, reliable detection of BTA for real-time monitoring of environmental samples. Given that BTA can be electrochemically reduced at low potentials, electrochemical detection on screen-printed electrodes (SPE) emerges as a promising approach. SPEs offer a more cost-effective, portable alternative to traditional electrochemical setups. In this work, a sensor based on carbon nanotube-Nafion-modified SPE is proposed for the detection of BTA. The electrochemical behaviour was evaluated via CV. BTA exhibited a single reduction peak around –1,4 V vs. Ag with no observable oxidation peak during the reverse scan. The SPE-C/SWCNT exhibited significant adsorption capacity for BTA. As a result, SWV analysis was performed after a 60 s preconcentration period at –1 V. With this approach a limit of detection (LOD) of 2 μM was calculated, which shows its potential for environmental monitoring.

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# Fabrication of solid oxide fuel cells

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Existing fossil fuel power units should be replaced with more efficient and environmentally friendly alternatives, such as fuel cells that can directly convert chemical energy into electrical energy. Solid oxide fuel cells (SOFCs) stand out due to their high efficiency and a wide range of usable fuels.

Our work includes the fabrication of anode-supported SOFCs by tape casting and screen printing, followed by sintering. A suspension of NiO and $Y_{0.08}Zr_{0.92}O_{1.96}$ (NiO-YSZ) powder mixture was tape-cast and laminated into a ≈400 μm thick sheet. The YSZ electrolyte, $Ce_{0.7}Gd_{0.3}O_{1.85}$ (GDC) protective layer and $La_{0.6}Sr_{0.4}Co_{0.9}Fe_{0.1}O_3$ (LSCF) cathode were screen-printed on the anode. The multilayer structure was sintered at 1400 °C in air.

Scanning electron microscopy (SEM) and focused ion beam microscopy (FIB) of the cross–section revealed no noticeable mechanical defects between individual layers, as seen in Figure 1a. Electron backscatter detection was also performed, showing clear boundaries between different materials and layers (Figure 1b).

We plan to use FIB-SEM tomography to create 3D reconstruction of the SOFC microstructure [1]. The topographic image of the microstructure will be used in finite element simulations to study the SOFC performance. The results of simulations will be validated and compared to experimental data.

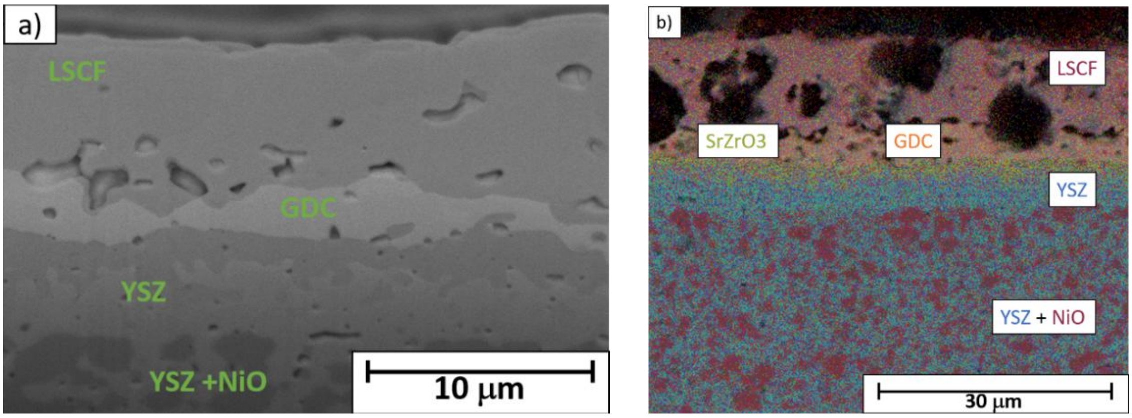

Figure 4: a) FIB analysis of the SOFC cross-section, b) EDS analysis of the SOFC cross-section.

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# Ruthenium-Doped Titanium Oxynitride-Based Immunosensor for the Sensitive Detection of Prostate-Specific Antigen (PSA)

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Prostate cancer affects approximately 1.4 million men worldwide each year [1]. In the European Union, it is the most common type of cancer in men and the third leading cause of cancer-related mortality [2]. Since the introduction of PSA testing, most prostate cancers have been detected at early stages, significantly improving survival rates [3]. Electrochemical sensors offer an alternative to traditional biochemical assays with several advantages, including fast response times, low production costs, point-of-care applicability, and high sensitivity [4].

In this work, we present an impedimetric immunosensor for the sensitive detection of PSA. The immunosensor is based on a novel (electro)catalytic material consisting of ruthenium-doped titanium oxynitride on a graphene support ($TiO_xN_y$-Ru-G). The material was silanized using (3-aminopropyl)triethoxysilane (APTES). We used a protocol for the chemical binding of anti-PSA antibodies with glutaraldehyde as a cross-linker and protein A (Figure 1). The (electro)catalytic activity of $TiO_xN_y$-Ru-G was demonstrated, as well as the ability of its APTES-modified form to suitably immobilize protein layers. The electroanalytical performance, characterized by high linearity over the investigated concentration range and a low detection limit, highlights the potential of this material in immunosensor development.

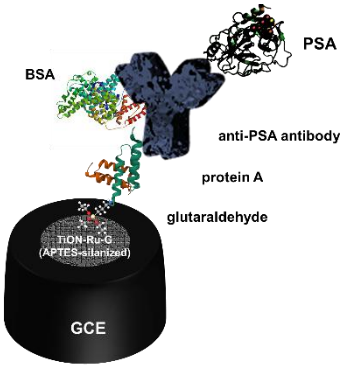

**Figure 1**. Architecture of the proposed immunosensor.

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## Acknowledgements

This research received funding from the Slovenian Research Agency: Research Program P1-0034, Research Projects J1-50019, P1-0153, and grant agreement no. 59876.

# MXene-Modified Impedimetric Genosensor for Sensitive Detection of Hop Pathogen

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*Citrus bark cracking viroid* (CBCVd) was first found in hops in 2007, pressing countries like Slovenia and Germany to seek early detection tools. CBCVd often shows no early symptoms, complicating timely identification, and since no treatment exists, infected plants must be removed, causing economic losses. Electrochemical methods provide a simple and cost-effective way to detect pathogens, though few studies focus specifically on viroids [1].

In this work, a sensitive, selective, and label-free impedimetric genosensor was developed for the detection of CBCVd in total RNA samples from hops. A glassy carbon electrode modified with streptavidin- agarose beads and $Ti_3C_2T_x$ MXene serves as an immobilization layer for biotinylated single-stranded DNA capture probes (Figure 1). After incubation with denatured total RNA hop extract, the capture probes hybridize with the CBCVd target sequences. Several fabrication and operating parameters were optimized, including the deposition time of the streptavidin agarose beads, the immobilization time and concentration of the capture probes, and the incubation time of the samples. The optimized genosensor showed excellent sensitivity with a detection limit of only 0.5 fg $\mu L^{-1}$ (5.5 fmol $L^{-1}$), eliminating the need for an additional nucleic acid amplification step [2]. The developed genosensor offers a rapid, cost-effective, and highly sensitive alternative for CBCVd detection. This approach could potentially improve disease management in hop cultivation, minimize economic losses and increase the sustainability of hop production.

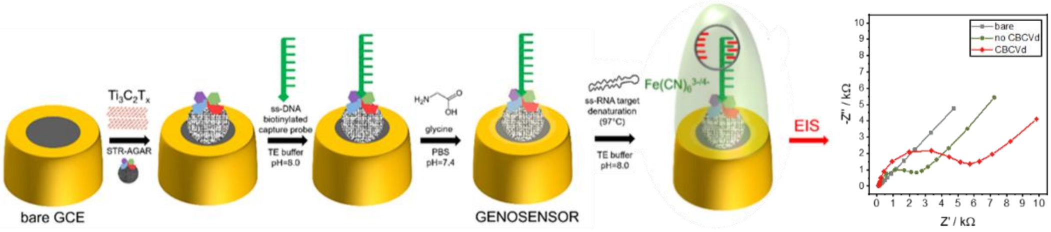

**Figure 5.** Graphical Abstract.

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Acknowledgments:

This research received funding from the Slovenian Research Agency (P1-0034, J1-3017, and grant agreement no. 56119).

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# Characterization of a novel plant virus found in irrigation water samples

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Tombusviruses are environmentally stable plant viruses with a narrow host range. They are primarily transmitted mechanically, without the need for biological vectors. These viruses are often found in environmental samples, such as water and soil, where they can remain infective for prolonged periods of time and can subsequently be directly transmitted to host plants. A novel virus, named Gorica tombusvirus 1, was initially discovered during a virome study of irrigation water sources in Slovenia. In that study a partial genomic sequence of this virus, lacking two open reading frames (ORFs) was reconstructed. Later, we detected Gorica tombusvirus 1 in a pooled plant sample collected near the wastewater treatment plant in central Slovenia. Here, we tested RNA extracts from individual plants included in the pooled sample and identified *Plantago lanceolata* as a possible host of this virus. Employing additional sequencing datasets containing this virus from this and other available studies we reconstructed extended genomic sequence of the virus, including two previously missing ORFs. Using global database data mining using Logan Search tool we detected Gorica tombusvirus 1 and reconstructed its genome from dataset originating from a river study done on New Zealand, suggesting a broader geographical distribution of the virus. Furthermore, to study its infectivity, host range and potential associated disease symptoms, we are currently conducting test plant bioassays including several species of test plants, including *Plantago lanceolata*, *Plantago major*, *Nicotiana benthamiana* and *Chenopodium quinoa*. This research contributes to the understanding of presence and diversity of stable plants viruses in environmental samples, such as river water, and their potential to infect wild or crop plants.

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# Monitoring of avian influenza viruses in environmental waters

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Zoonotic diseases—infectious diseases transmitted between animals and humans—account for approximately 75% of emerging infectious diseases, posing a significant global health and economic threat. Among these, avian influenza is recognized as a top-priority zoonotic threat [1]. Avian influenza viruses (AIVs), part of *Orthomyxoviridae*, can infect a broad range of wild avian and mammalian species, including humans, where they may cause severe illness and high mortality rates [2]. These viruses circulate among different hosts and are also excreted into the environmental waters [3], which we aim to use as surveillance tool. Our aim is to develop and optimize methods for detecting AIV in surface water and sediment, within the framework of the so-called water-based epidemiology. This approach offers an alternative to traditional active surveillance methods that rely on capturing or sampling wild birds. Monitoring is being conducted at two sites—Lake Zbilje and Reservoir Medvedce, key migratory waterbird habitats with a history of AIV presence.

Due to the extremely low abundance of viruses in environmental waters, various concentration methods will be evaluated, including large-volume concentrator (LVC) combined with concentration pipette (CP) Select (both Innovaprep), CIM monolith chromatography (Sartorius), traditional adsorption to electropositive membranes (Millipore), and passive samplers called torpedoes. Detection of viral genomic RNA will be performed using two RT-qPCR assays, a generic one targeting influenza A, and a more specific one targeting the H5 subtype. Positive samples will undergo whole-genome sequencing for subtype characterization and identification of mutations or reassortment events—key drivers of viral evolution and potential pandemics.

As the risk of spillover events from wildlife continues to rise, environmental surveillance offers a vital tool for pandemic preparedness and global health security. We will confirm whether integrating it with traditional monitoring can enhance early detection and tracking of AIV circulation.

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# Polarization Mapping in Potassium Sodium Niobate by 4D STEM, Multi-Slice Simulations, and First-Principles Calculations

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Four-dimensional scanning transmission electron microscopy (4D STEM) is an advanced microscopy technique that captures a 2D diffraction pattern at each probe position in a 2D raster scan. Unlike conventional STEM, which collects only integrated signals, 4D STEM provides significantly richer and more detailed structural data, including electric and magnetic strain distributions, charge density distribution, and other structural properties [1].

In this study, we employ atomic-scale 4D STEM to investigate ferroelectrics, specifically lead-free $(K_{0.5}Na_{0.5})NbO_3$ (KNN), a subclass of piezoelectrics that exhibit spontaneous electric polarization, which can be reversed by an external electric field. Understanding the distribution, direction, and magnitude of spontaneous polarization is essential for gaining deeper insight into the fundamental properties of these materials.

Samples for 4D STEM analysis were prepared using conventional method, including grinding, polishing, dimpling and Ar ion milling. 4D STEM datasets of bulk KNN were acquired using a Cs-corrected ARM200CF (Jeol, Tokyo, Japan) equipped with a Merlin pixelated detector (Quantum Detectors, Oxford, UK). 4D STEM diffraction patterns were simulated using QSTEM program (C. Koch, PhD thesis, Arizona State University, 2002). Charge density distribution was calculated using first-principles DFT calculations with Quantum ESPRESSO.

KNN's orthorhombic symmetry allows 12 possible Nb displacement directions, corresponding to the spontaneous polarization direction. Along the $[100]_{pc}$ zone axis, Nb shifts in one of 8 distinct directions from its centrosymmetric position. 4D STEM simulations show that Nb atoms displace in the opposite direction to oxygen. Experimental 4D STEM results will be compared with DFT calculations, QSTEM simulations and discussed.

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# Stabilization Strategies for Prussian Blue Electrodes in Polyamine Sensing Applications

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Polyamines (PAs) spermine, spermidine and putrescine, play vital roles in cellular functions and are tightly regulated by homeostasis. Their abnormal concentration is closely linked to various health conditions, including neurodegenerative diseases and cancer. Therefore, accurate PA monitoring in biological fluids such as saliva and urine is essential for both diagnostic and therapeutic purposes. While traditional chromatographic analysis offers high sensitivity and reliability, it is unsuitable for point-of-care applications due to its complexity, cost, and lack of portability. In recent years, electrochemical biosensors have emerged as a promising alternative for real-time PA monitoring, offering rapid analysis, miniaturization potential, and compatibility with portable devices.

Because PAs cannot be directly detected due to electrochemical inactivity, most existing PA sensors integrate Prussian blue (PB) with polyamine oxidases. These enzymes catalyse the oxidation of PAs, generating hydrogen peroxide ($H_2O_2$), which is then detected electrochemically via the PB layer. Known for its exceptional electrocatalytic activity and selectivity for $H_2O_2$ reduction, PB functions as an artificial peroxidase, enabling $H_2O_2$ detection at low applied potentials around 0 V vs. Ag/AgCl.

However, the stability of the PB layer in biological fluids at neutral pH is limited, reducing its activity and shortening the sensor's operational lifespan. To address this challenge, various approaches have been explored to enhance the stability of the redox mediator layer, including optimization of the synthesis method and the incorporation of nanomaterials and polymers.

The present study investigates different synthesis approaches for fabricating PB-modified carbon screen-printed electrodes, focusing on how these methods affect the stability of the PB layer during $H_2O_2$ sensing in phosphate-buffered saline (PBS). Additionally, it evaluates the binding performance of several polymers, including polyaniline, polyvinylpyrrolidone, polydiallyldimethylammonium chloride, and chitosan. Our results demonstrate that incorporating a conductive polymer effectively minimizes material loss while maintaining the sensor's sensitivity to $H_2O_2$.

# Investigation of the piezoelectric properties of ceramic powders using piezo-response force microscopy

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Piezo-response force microscopy (PFM) is widely used to analyze piezoelectric and ferroelectric properties in various materials such as single crystals, bulk ceramics, thick and thin films and also nanoobjects. However, the investigation of ceramic powders with PFM is challenging due to their irregular non-flat shape, weak attachment to the substrate and movement of particles during PFM scanning. Given these challenges, it is necessary to develop a new procedure for investigating ceramic ferroelectric powders using PFM. In this study, ceramic powders were analyzed using PFM. In order to prevent particles movement and sticking to the PFM tip, the powders were embedded in epoxy resin and polished using standard metallographic techniques, finishing with a colloidal $SiO_2$ suspension with particles only a few tens of nanometers in size. The samples were placed in a custom holder with the polished surface facing up. A bias voltage with an amplitude of 5 V and frequency of 278 kHz was applied to the PFM tip in the virtual ground mode (schematically shown in Figure 1a). Vertical PFM images (Figure 1b) and local hysteresis loops (Figure 1c and d) were obtained in a dual ac-resonance switching spectroscopy mode using MFP-3D AFM. Ferroelectric $PbZr_{0.53}Ti_{0.47}O_3$ (PZT) powders were investigated in this work. The PFM amplitude image of PZT powder (Figure 1b) reveals piezoelectric activity. In larger particles ferroelectric domains are visible. To analyze polarization switching within individual particles, local piezo-response hysteresis loops were measured at the yellow-marked location in Figure 1b. The amplitude and phase loops (Figures 1c and d) confirm ferroelectric domain switching within a single particle.

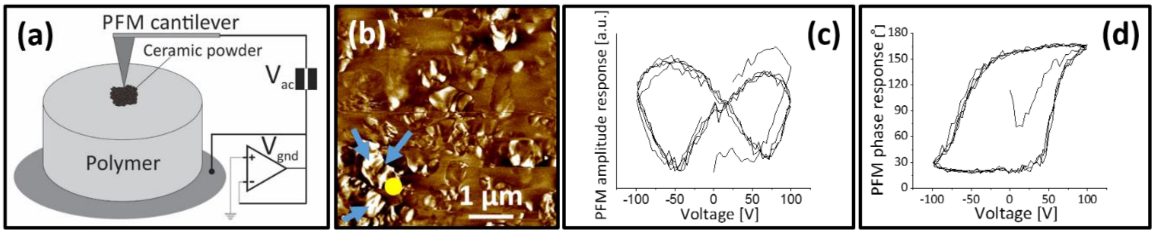

**Figure 1**. (a) Scheme. (b) PFM amplitude image. PFM (c) amplitude and (d) phase hysteresis loops.

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