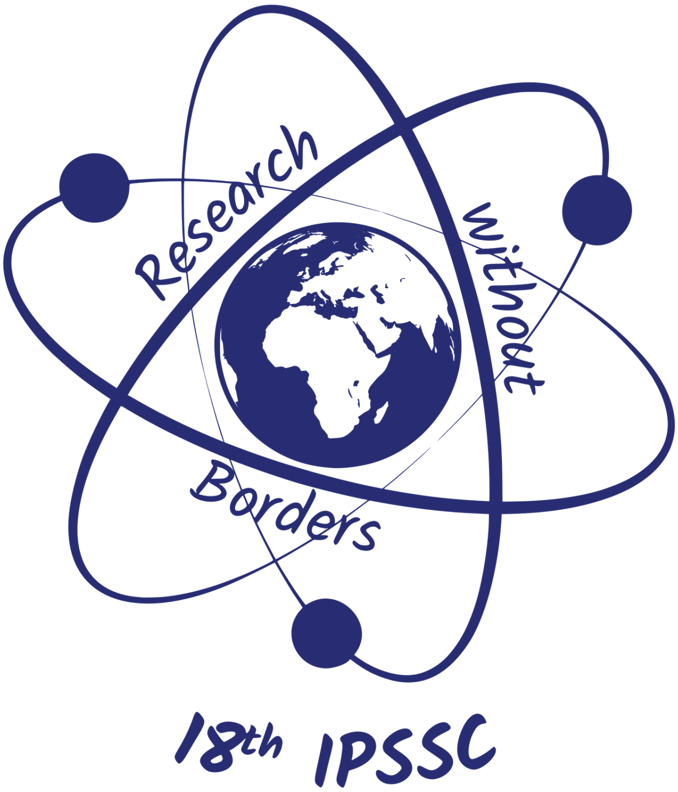
BOOK OF ABSTRACTS



18th Jožef Stefan
International Postgraduate School
Student's Conference

18th Jožef Stefan International Postgraduate School Students' Conference

Book of abstracts

Edited by:

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Contents

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IPS Student Council

This year, the 18th Jožef Stefan International Postgraduate School Students' Conference was held at Miren Castle from 27 to 29 May 2026. The theme of the conference was Research without Borders. With this theme, we wanted to emphasize that modern research often goes beyond the limits of a single discipline, method, institution, or country. Many of today's scientific problems require collaboration between different fields, from experiments and modelling to data science, artificial intelligence, advanced materials, environmental research, and sensor technologies.

The invited programme reflected this idea from several perspectives. Richard Wheeler and Robert Zorec opened the conference with the lecture Career Planning and Becoming a Great Scientist and later joined the Ask Me Anything session, where students could discuss research, careers, creativity, and scientific work in a more informal way. Richard Wheeler also gave a lecture titled What is AI Really, and What are the Scientific Jobs of the Future, connecting current developments in AI with the future of research. Together with Robert Zorec, he also led the Student Pitch Session, where students presented their research ideas and received direct feedback.

The conference also included contributions from industry and applied research. Matej Kalc from NLB presented AI Engineering at NLB, showing how AI is used in practical applications. Darko Delgalo from KemoLab introduced Vacuum and Analytical Technologies at KemoLab, while Rok Novak gave a lecture on Public Speaking in Science, focusing on how researchers can present their work more effectively.

As always, the main part of the conference was the student programme. This year, students contributed numerous oral presentations and took part in three poster sessions. The topics covered a wide range of research areas, including information and communication technologies, nanosciences and nanotechnologies, ecotechnologies, and sensor technologies. The diversity of the programme showed how much high-quality and interdisciplinary research is being carried out by young researchers at MPŠ and partner institutions.

The conference was prepared by the IPS Student Council and the Student Conference Organizing Committee, with the support of the Dean of IPS, Prof. Dr. Milena Horvat, Prof. Dr. Aleksander Zidanšek, Sergeja Vogrinčič, Tadeja Samec, mentors, reviewers, and everyone else who contributed to the organization. Their work made it possible to create a well-organized student-led event and an open space for scientific exchange.

We also thank our sponsors and supporters: the Jožef Stefan International Postgraduate School, the Jožef Stefan Institute, Istrabenz plini, ITR-LAB, NLB, KemoLab, Trimo, SCAN, Chemass, Kolektor, Akrapovič, ACO, Avtotehnika Celje, the National Institute of Biology, Bird Buddy, Petrol, KIMI, ŠOU Ljubljana, Krka, Telekom Slovenije, and Red Bull, as well as all others who supported the conference.

We hope that IPSSC 2026 encouraged participants to look beyond the usual borders of their own research fields, build new connections, and continue developing as independent young scientists.

Juš Polanšek, Sebastian Mežnar, and Martina Žabčić
on behalf of the IPS Organizing Committee and the IPS Student Council

Foreword from the Dean

This Book of Abstracts brings together the contributions presented at the 18th Jožef Stefan International Postgraduate School Students' Conference (IPSSC). It is a record of research in progress, but also a reflection of something equally important: the independence, initiative, and maturity of the students who shaped this conference.

IPSSC has a special place in the life of the School because it is not only a conference for students, but also a conference created with students and, to a large extent, by students. The Student Council, together with other highly engaged students, has taken an active role in preparing an event that responds to the needs, interests, and expectations of young researchers. Their work shows organisational ability, responsibility, cooperation, and a genuine care for the academic community.

This year, we are especially pleased that the conference has also welcomed students from outside MPŠ. Their participation brings additional perspectives, broadens the exchange of ideas, and strengthens the role of IPSSC as an open meeting place for young researchers.

The theme of this year's conference, *Research without Borders*, is therefore more than a title. It speaks to the kind of science we need today, and to the kind of research environment we try to build at MPŠ. Research without borders means crossing the borders between disciplines, where complex questions require knowledge from different fields. It means crossing the borders between countries, through international collaboration and openness to different perspectives. It also means crossing the borders between academia and society, so that research remains connected to real technological, environmental, and social challenges.

At the same time, research without borders invites us to move beyond the borders between methods and approaches. Modern science brings together experiments, modelling, data science, artificial intelligence, advanced analytics, and many other tools. It also reminds us that fundamental and applied research are not separate worlds, but parts of the same search for understanding and meaningful contribution.

The abstracts collected in this volume show the breadth of research carried out by our students in Ecotechnologies, Nanosciences and Nanotechnologies, Information and Communication Technologies, and Sensor Technologies. They also show the curiosity, persistence, and growing confidence of young researchers who are finding their own scientific voice.

I would like to thank all authors, mentors, reviewers, members of the Student Council, and everyone who contributed to the preparation of this conference. I also sincerely thank our sponsors, whose support helps make this student-led event possible and contributes to its quality, openness, and visibility. On behalf of the Jožef Stefan International Postgraduate School, I wish all participants a successful and inspiring conference.

Prof. Dr. Milena Horvat
Dean
Jožef Stefan International Postgraduate School

Ecotechnologies

Method development for separation and purification of Ag-111 from neutron irradiated Pd targets

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Modern applications of radiopharmaceuticals utilize theranostic nuclides for simultaneous diagnosis/imaging and treatment of tumors. Ag-111 is a promising candidate for this field, due to its advantageous decay properties. The beta particles emitted ($E_{\beta,mean}$=360 keV) interact primarily with cancer cells, while concurrent emission of gamma rays (245, 342 keV) enables the possibility for imaging with techniques like Single Photon Emission Computed Tomography (SPECT). Ag-111 is produced mainly in nuclear reactors via neutron activation of the stable Pd-110 isotope present in natural palladium targets. Nonetheless, the challenging Ag/Pd separation can have a negative impact on several quality parameters of the final product, such as total activity and radiochemical or radionuclidic purity. Moreover, the relatively low isotopic abundance of Pd-110 (11.72 %) dictates the need for costly isotopically enriched targets, and, thus, for recovery and recycling protocols. This study was focused on the development of quick and efficient procedures regarding Ag/Pd separation and consequent palladium recovery. Natural palladium targets of up to 20 mg were neutron irradiated at the TRIGA MARK II research reactor at Jožef Stefan Institute for up to 12 h (maximum flux 3.9E+12 $cm^{-2}s^{-1}$), followed by assessment of yield and impurities by gamma spectroscopy. Separation protocols were developed, studied with non-radioactive materials and mass spectrometric measurements, and finally validated with irradiated targets, to isolate Ag-111. Separation was investigated using both the chromatographic Ni Resin, and only dimethylglyoxime (DMG), the active component of the resin, which selectively reacts with Pd(II) ions. Method efficiencies and yields were then evaluated and compared. Finally, the dissolved Pd was recovered almost quantitatively through reduction with ascorbic acid. The results of this study indicate that the protocols applied can be used for the efficient separation and purification of Ag-111, and for the recovery of the target for prospective additional irradiation cycles.

A Multi-Disciplinary Workflow for the Non-Destructive Restoration of Stone Heritage

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Conservation of cultural heritage objects may be challenging when artefacts suffer from internal structural decay, including hidden voids, material heterogeneity or deep fracture networks. Surface-level 3D scanning cannot detect these internal features or identify previous incompatible restoration materials, such as cement-based mortars, which can accelerate long-term deterioration. This study develops a non-destructive workflow to assess internal damage and support the design of compatible restoration materials.

A sculptural head from Dornava, Slovenia, served as the primary case study. The clay reconstruction of the head of the statue of the Immaculate Mary is part of an extensive conservation and restoration project aimed at preserving the stone sculptures at the Baroque Dornava Manor, a monument of national importance. We combined handheld structured-light 3D scanning with multi-scale X-ray computed microtomography (XμCT) to document both surface morphology and internal structure. The XμCT analysis revealed fracture propagation, allowing the identification of structurally critical zones requiring stabilization. These volumetric datasets informed the development of optimized digital models for powder bed additive manufacturing. Additive manufacturing is used to produce customized molds for casting geopolymer binders, ceramic-like materials selected for their chemical compatibility and suitable rheological properties.

The volumetric datasets were used to develop optimized digital models suitable for powder bed additive manufacturing. Additive manufacturing is currently being applied to produce customized molds designed for casting geopolymer binders, ceramic-like materials selected for their chemical compatibility with the original material and their suitable rheological properties. Particular attention is given to the reconstruction of fragile morphological features, such as the nasal bridge and undercut areas around the lips and eyelids.

The ongoing research aims to validate a reproducible reverse-engineering workflow for cultural heritage conservation. The results are expected to contribute to the development of sustainable and compatible restoration techniques applicable to complex heritage objects.

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Detection of contaminants of emerging concern with targeted and non-targeted analysis applied to hair samples

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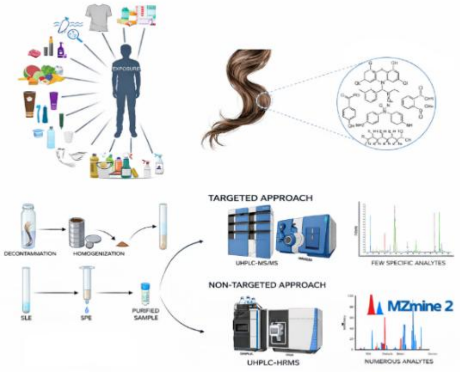

Figure 1: Determination of exposure biomarkers in hair.

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 represents an alternative, non-invasive matrix that offers a broader exposure window due to the gradual accumulation of xenobiotics over time. Current research in hair biomonitoring mainly focuses on the detection of elements, drugs, or structurally related groups of exposure biomarkers (BoEs). To our knowledge, neither wide-scope targeted analysis nor non-targeted screening (NTS) approaches have yet been systematically applied to the analysis BoEs in human hair. My PhD project will focus on the development of an NTS method for wide-range detection of BoEs in human hair samples, building on the in-house method previously validated for targeted analysis. As a step towards the broader implementation of hair in HBM we plan to conduct an interlaboratory comparison involving expert laboratories from Slovenia, France, Italy, Denmark and the Netherlands. The results of this exercise could provide an important basis for development of SOP, and, in the longer term, support the development of the first CRM for hair. The applicability of the developed approach will be demonstrated on real samples collected from different geographical regions in Europe, enabling the exploration of differences in exposure pattern across European populations. This study aims to provide the first biomonitoring of BoE in hair using NTS. It will contribute to advancing exposure assessment using non-invasive matrices, support biomarker prioritization for future biomonitoring campaigns, and potentially enable the identification of early-warning signals related to emerging chemical exposures.

Pesticide residues in honey, bees and pollen

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The extensive use of pesticides poses a significant threat to ecosystems and human health. Although seasonal and geographical variability in pesticide contamination have been reported, the relationship between residues detected in hive products and bees remains insufficiently understood. In this study, a multiresidue analytical method was developed and validated for the determination of 60 pesticides in bees, honey, and pollen. The method combines the QuEChERS (Quick, easy, cheap, effective, rugged, and safe) extraction followed by liquid chromatography tandem mass spectrometry (LC-MS/MS). The method validation results demonstrated matrix-matched calibration with correlation coefficients higher than 0.989. The recovery ranged from 73.4% to 120%, with the strongest matrix effect observed in honey, followed by bees and pollen. The limits of quantification ranged between 0.1 and 10 ng/g, with the inter-day precision below 20% RSD. Sampling was conducted at four Slovenian apiaries located in different environments including agricultural fields (Nova Gorica), urban areas (Ljubljana–Veterinary Faculty), mountainous with open land (Vremščica), and valley forest areas (Prevalje). Sampling was performed during both spraying and non-spraying seasons. A total of 30 pesticides were detected across the analysed matrices. Among these, 21 were detected during the spraying season, 4 during the non-spraying season, and 5 in both periods. Pesticides were most frequently detected in bees, while pollen contained most diverse pesticides. The highest contamination levels were observed in Nova Gorica, and the lowest was found in Prevalje. Overall, this study shows that honey bees and their products can serve as bioindicator of pesticide exposure, revealing clear seasonal patterns and regional contamination. In this respect, the study improves our understanding of pollinators and their associated environmental risks across different locations.

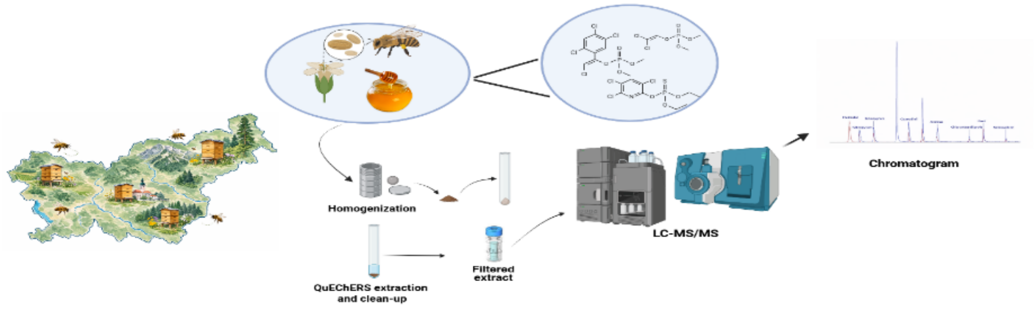

Figure 2: Dynamic Schematic overview of the study workflow

Genetic polymorphisms impacting urinary metabolites of polycyclic aromatic hydrocarbons in Slovene general population

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Polycyclic aromatic hydrocarbons (PAHs) are compounds with documented harmful effects containing multiple aromatic benzo rings fused together. This study utilizes participants of the second national human biomonitoring programme in Slovenia (SLO-HBM-II), which focuses on primary school pupils sampled between 2018 and 2024 in nine different areas across the country to investigate whether single-nucleotide polymorphisms (SNPs) can affect the levels of PAH metabolites in urine. To identify polymorphisms of interest, we combined a literature search on PAH metabolism and correlations between PAH levels and selected SNPs in participants from the first national human biomonitoring programme (SLO-HBM-I), which focused on men and primiparous lactating women aged between 18 and 49 years. To account for possible confounders, the statistical analysis was performed separately for men and women and adjusted for potential dietary and lifestyle factors, as well as blood levels of essential elements (copper, zinc, selenium) and serum TSH levels. Based on the results, the SNPs of genes with potential interaction with PAH exposure were identified as follows: delta-aminolevulinic acid dehydratase (ALAD; rs1800435, rs818684 and rs2761016), cytochromes P450 and uridine glucuronyl transferase (CYP2C9 rs1799853, CYP2C19 rs12248560, CYP2D6 rs3892097 and UGT1A7 rs11692021). Literature cites CYP450 and UGT enzymes as PAH metabolizers, while ALAD helps synthesize heme, a component of CYP450 enzymes, supporting a potential involvement in PAH metabolism in the body. Genotyping of these genes will also be performed in the DNA isolates from children and adolescents across Slovenia (n=1787) and the obtained allele annotation will be used in the statistical models to re-evaluate the most significant factors influencing exposure to PAHs in comparison with the adult population. With this study, we hope not only to make a step forward in establishing susceptibility markers for PAH exposure in human biomonitoring, but also expand the current knowledge on PAH toxicokinetics in the human body.

Reactivity of [PhC(NtBu)$_2$]Si(=Se)Cl toward halogenating reagents

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Amidinate-stabilized low-valent silicon compounds represent an important class of highly reactive species capable of forming multiple bonds with chalcogens [1,2]. Compounds containing a Si=Se fragment are of particular interest as heavier analogues of the well-studied C=Se systems. While the reactivity of C=Se double bonds toward halogens has been extensively investigated [3], analogous transformations of Si=Se systems remain significantly less explored.

In this work, the reactivity of the [PhC(NtBu)$_2$]Si(=Se)Cl toward different halogenating reagents was investigated. SO_2Cl_2 and $SOCl_2$ were used as sources of Cl_2 and Cl^-, respectively, while Br_2 and I_2 were employed as molecular halogens. The reactions were carried out in CH_2Cl_2 at room temperature. The reaction mixtures and isolated products were analyzed by NMR spectroscopy, and the structures of the obtained compounds were confirmed by single-crystal X-ray diffraction. Reaction with $SOCl_2$ leads to the formation of [PhC(NtBu)$_2$]$SiCl_3$, indicating cleavage of the Si=Se bond and chlorination at the silicon center. In contrast, treatment with SO_2Cl_2 results in the formation of ionic products containing $[SeCl_6]^{2-}$ anions. Reaction with I_2 produces salts containing the polyhalide anion I_3^-, with the product composition depending on the amount of iodine used. In the case of Br_2, changes in the NMR spectra were observed, and formation of a bromide salt of the ligand was detected.

These results show that reactions of [PhC(NtBu)$_2$]Si(=Se)Cl with halogenating reagents lead to cleavage of the Si=Se bond and formation of ionic halogenide species.

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Reducing sample heterogeneity contribution to measurement uncertainty in total and methylmercury determination in fish tissue

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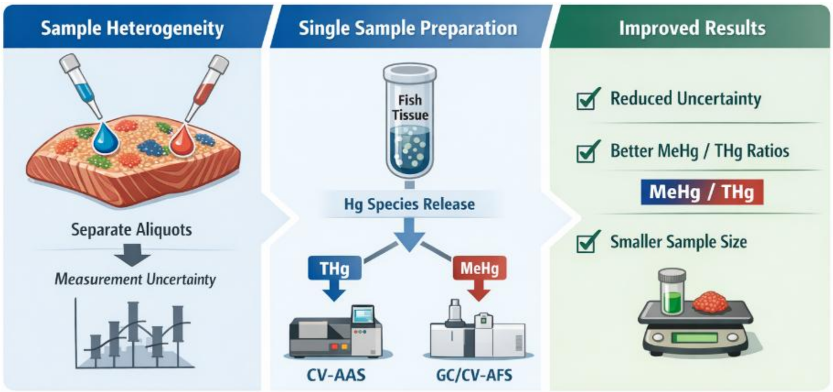

Figure 1. Graphical abstract

Fish consumption is the main source of human exposure to methylmercury (MeHg), which usually represents more than 85% of the total mercury (THg) present in large predatory fish. Reliable determination of the MeHg fraction is therefore essential not only for assessing mercury exposure and understanding mercury bioaccumulation in aquatic ecosystems, but also for understanding the adaptation of fish to environmentally stressed habitats, where the proportion of MeHg can provide important additional insight. For this reason, the first aim of this work was to validate the analytical procedures and ensure the most reliable results possible. To reduce the influence of sample heterogeneity, which can compromise comparability when THg and MeHg are determined from separate aliquots, we adapted a conventional approach to enable the determination of both species from the same sample aliquot. After releasing THg and MeHg from the biological matrix, total mercury was measured by cold vapour atomic absorption spectrometry (CV-AAS), while methylmercury was determined after acid digestion using gas chromatography coupled with cold vapour atomic fluorescence spectrometry (GC/CV-AFS). The method was tested using two certified reference materials from the National Research Council of Canada, dogfish liver DOLT-3 and DOLT-5. MeHg was quantified using a multi-point calibration curve prepared from working calibration solutions, while inorganic mercury and THg mass balance were evaluated using a second calibration based on the NIST 3133 mercury standard. The proposed approach significantly reduces uncertainty related to sample heterogeneity, improves the reliability of MeHg/THg ratios, and requires smaller sample amounts. It therefore offers a practical solution for mercury speciation analysis in biological samples, especially when sample availability is limited.

Selective recovery of zinc using deep eutectic solvents

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Steelmaking generates millions of tonnes of electric arc furnace dust (EAFD) annually. EAFD is classified as hazardous waste and its high zinc content (up to 30%) makes it a valuable secondary resource of zinc. Current recycling methods are energy-intensive and have a significant ecological footprint [1]. A promising approach is the use of deep eutectic solvents (DES), a class of “green”, tunable, low-cost and non-toxic liquid salts, as a sustainable alternative for selective zinc extraction [2]. Six choline chloride-based DES were synthesised using different hydrogen bond donors, including urea, ethylene glycol, fructose, and various organic acids (levulinic, malonic, and oxalic). Using a Taguchi experimental design, we evaluated the influence of temperature, time, and liquid-to-solid ratio on the leaching of two mineralogically different industrial EAFDs. Our results showed that metal recovery is highly dependent on solvent composition: amide-based DES (urea) provide near-perfect selectivity by leaving the iron matrix intact, although zinc recovery is limited to 50%. In contrast, organic acid-based DES achieve much higher zinc recovery (60–80%) but exhibit lower selectivity. Statistical analysis identified temperature and the liquid-to-solid ratio as the most influential process parameters, depending on DES composition. The results demonstrate that tailored DES can compete with conventional sulphuric acid leaching in efficiency and may provide superior selectivity. This study highlights the currently under-investigated potential of green solvents for sustainable metallurgical processes and emphasises the crucial role of solvent composition and leaching conditions in achieving optimal and selective zinc recovery.

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Multi-element and Lead Isotope Analysis of Contamination in Slovenia's Meža and Drava River Systems

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Potentially toxic elements (PTEs) are environmentally persistent and can accumulate in the biotic environment, posing risks when present at elevated concentrations. They originate from both natural processes and anthropogenic activities, particularly mining and smelting. The Meža Valley (Slovenia) is an example of long-term contamination, primarily with lead (Pb), resulting from extensive historical mining dating back to Roman times and peaking in the mid-20th century. During this period large quantities of mine waste that contained high concentrations of Pb and other PTEs were deposited in the area, which led to contamination of the Meža River and its tributaries, and extending downstream into the Drava River system.

Effective mitigation of such contaminants requires a detailed understanding of how PTEs move through the environment and how they reach and affect living organisms. However, the complexity of PTE cycling, including dissolution, sorption, remobilisation, and biological uptake, means that concentration data alone are insufficient to identify pollutant sources or predict environmental behaviour. Accordingly, the DISCOVER project was initiated to develop advanced analytical methods for studying sources, behaviour, and fate of PTEs, present in the contaminated Meža Valley environment, integrating elemental, isotopic, and nanoparticle approaches.

This study aims to characterise the spatial and temporal distribution of PTEs across the Meža and Drava river systems. The objectives are to: (1) determine concentrations and spatial patterns of PTEs in sediments, water, and biota along the contamination gradient; (2) assess whether Pb isotope ratios can differentiate between pollution sources and reflect both historical and ongoing inputs; and (3) establish geochemical linkages between sources and environmental sinks in the catchment.

The results will improve understanding of PTE mobility, bioavailability, and transfer through ecosystems, including potential uptake by plants and humans, thereby contributing to crucial information for environmental and human health risk assessment in the Meža and Drava catchments.

Deficit irrigation modulates the concentration of 3-sulfanylhexan-1-ol in Pinela (*Vitis vinifera* L.) wines

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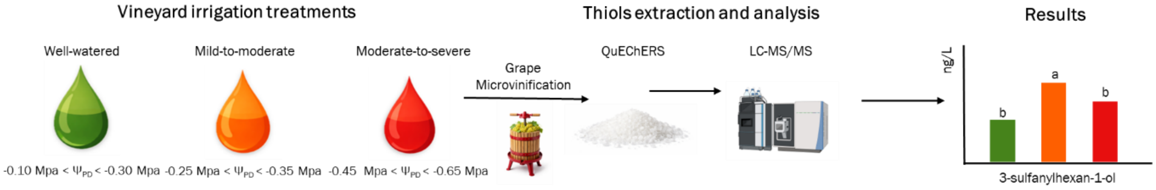
Varietal thiols contribute positively to tropical aroma of wines. The main thiols in wines are 4-methyl-4-sulfanylpentan-2-one (4MSP), 3-sulfanylhexan-1-ol (3SH), and 3-sulfanylhexylacetate (3SHA) [1]. Despite their low concentration, they are potent odorants due to their low perception threshold: 0,8 ng L^{-1} for 4MSP, 60 ng L^{-1} for 3SH and 4,2 ng L^{-1} for SHA.

As far as we know, only one study has reported their presence in Pinela wines, and ours is the first that discusses the influence of deficit irrigation on thiol formation in Pinela wines.

The experiment was conducted during the 2024 vintage in a terraced vineyard in the Sub-Mediterranean climate of the Vipava Valley (Slovenia). Plant water status was monitored by predawn water potential (Ψ_{PD}) measurements from berry set to harvest. Three irrigation regimes were applied: well-watered control (−0.10 to −0.30 MPa), mild-to-moderate deficit (−0.25 to −0.45 MPa), and moderate-to-severe deficit (−0.45 to −0.65 MPa). Grapes were microvinified with commercial *Saccharomyces cerevisiae*. Concentrations of 4MSP, 3SH and 3SHA in wines were determined using a QuEChERS based method with LC-MS/MS [1]. Statistical differences were tested by ANOVA ($\alpha = 0,05$).

The concentration of 3SH in Pinela wines was significantly higher under mild-to-moderate vine water stress compared with both the well-watered and moderate-to-severe treatments. Mean concentrations were 676 ± 53 ng L^{-1} in the well-watered treatment, 848 ± 37 ng L^{-1} under mild-to-moderate stress, and 765 ± 76 ng L^{-1} under moderate-to-severe stress. In contrast, no significant differences were observed for 3SHA. 4MSP was not detected under any treatment.

Pinela wines were characterized by the presence of the varietal thiols 3SH and 3SHA above their perception thresholds. Irrigation significantly influenced 3SH levels, with the highest concentration observed under mild-to-moderate water stress.



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Advanced Saffron Origin Authentication Through Machine Learning and Isotopic–Elemental Fingerprinting

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Food fraud continues to threaten consumer confidence and the reliability of global food systems. To support more reliable saffron authentication, this study combines stable isotope ratio analysis and multi-element profiling with machine learning techniques. A dataset of 115 authenticated saffron samples originating from Iran, Italy, Morocco, and Spain was examined using 47 chemical features, consisting of 5 stable isotope ratios and 42 elemental concentrations. Four ensemble learning algorithms—Random Forest, XGBoost, LightGBM, and CatBoost—were assessed through stratified cross-validation combined with Bayesian hyperparameter optimization. Among the tested models, LightGBM applied to the combined isotopic and elemental dataset achieved the highest classification performance, reaching 93.1% accuracy, 90.1% balanced accuracy, and an F1 score of 0.934, indicating strong predictive capability even in the presence of class imbalance. Model interpretation using SHAP values showed that elemental variables, particularly nickel and cobalt, played the most important role in distinguishing geographical origins, whereas stable isotope ratios contributed relatively little to the predictions. These findings highlight the superior utility of multi-elemental analysis for cost-effective food authentication, supported by an interpretable and scalable machine learning framework, while stable isotopes, though less dominant in prediction, remain essential for grounding origin differences in environmental and regional context.

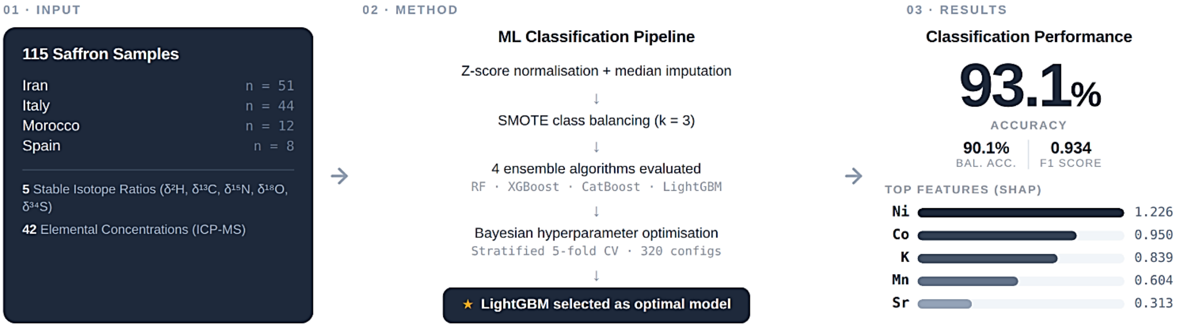

Figure 1: ML pipeline for saffron origin classification

XeF_2 competing with weakly coordinating anions in the coordination sphere of metal complexes

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XeF_2 can act as a ligand in coordination compounds with the general formula $[M(XeF_2)_n](WCA)_m$, where "M" is a metal center and WCA represents a weakly coordinating anion (AF_6^- (A = As, Sb, Bi, Ru, Ir,...), BF_4^-, $OTeF_5^-$) [1]. Until recently, it was believed that Ni as a metal center could not form such compounds, since Ni^{2+} was considered a sufficiently strong Lewis acid to withdraw fluoride ion from XeF_2, forming NiF_2 and $[XeF][AF_6]$ salts [2]. Nevertheless, in 2023 the first compound containing Ni as the metal center and XeF_2 as a ligand, $[Ni(XeF_2)_2](IrF_6)_2$, was synthesized [3]. We therefore extended our research to combinations with other anions of the type AF_6^- and prepared several new nickel compounds: $[Ni(XeF_2)_2](RuF_6)_2$, $[Ni(XeF_2)_6](RuF_6)_2$, $[Ni(XeF_2)_2](AsF_6)_2$, $[Ni(XeF_2)_4](AsF_6)_2$, $[Ni(XeF_2)_2](BiF_6)_2$, and $[Ni(XeF_2)_6](BiF_6)_2$ [4]. In addition to anions derived from the Lewis acids AF_5, we aimed to prepare compounds with other weakly coordinating anions, for example $CF_3SO_3^-$ (triflate anion). It turned out that in certain compounds, such as $Ca(CF_3SO_3)_2$, $CF_3SO_3^-$ coordinates too strongly to be displaced from the coordination sphere by XeF_2. Therefore, we tried to prepare more weakly coordinating anion. In a reaction mixture with HF as the solvent, we combined a Lewis acid with $Ca(CF_3SO_3)_2$, expecting the Lewis acid to bind $CF_3SO_3^-$ and form the species $Ca(AF_5CF_3SO_3)_2$. However, the addition of AsF_5 in HF yielded $Ca(SO_3F)(AsF_6)$, while the addition of BiF_5 resulted in $Ca(HF)(SO_3F)(BiF_6)$. We extended experiments to other triflates and have so far succeeded in preparing $Ba(SO_3F)(BiF_6)$. This synthetic route enables the preparation of compounds with mixed anions. We characterize them by Raman spectroscopy, NMR and XRD. Future research will focus on synthesizing additional mixed-anion compounds and as the main objective, preparing compounds with the general formula $[M(XeF_2)_n(SO_3F)](AF_6)$. Such compounds would represent the first coordination complexes containing XeF_2 as a ligand with a mixed-anion system.

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Dynamics of air infiltration rates affected by meteorological conditions in a residential building

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Air infiltration refers to the unintentional entry of outdoor air into a building through cracks, gaps, and other leakage paths. This is a dynamic process, largely affected by meteorological conditions, particularly outdoor air temperature, pressure and wind velocity. In our study, we examine the dependence of air infiltration rate (N_{inf}, h^{-1}) on meteorological conditions in a selected low-airtight building in an urban area. The study was conducted using continuous monitoring (30 min intervals) of CO_2 in a room under closed conditions and meteorological parameters (outdoor air temperature, pressure, and wind velocity) from December 2024 to February 2025. N_{inf} was determined for two temperature-based clusters: C1 (T_0=–5.4–4.8 °C), C2 (T_0=5.4–12.7 °C). In C1, N_{inf} shows a greater decrease during the first four hours (0.26–0.19 h^{-1}), when T_0 rises (–0.2–3.1 °C), while in C2, it is lower by a factor of 2.3 (0.20–0.17 h^{-1}) due to higher T_0 (6.5–9.2 °C). From 12:30 to 16:00, N_{inf} continues to decrease in both clusters, with the more pronounced change in C1 (0.19–0.16 h^{-1}) than in C2 (0.17–0.15 h^{-1}). This pattern is consistent with the slight increase in T_0. Correlation analysis confirms that T_0 is the main factor influencing N_{inf}, with the very high correlation coefficient in C1 (r=–0.91 to –0.96) and moderate to high in C2 (r=–0.61 to –0.95). Pressure and wind velocity showed weaker relationships. In low-airtight buildings, N_{inf} shows significant diurnal variations, which affects IAQ, particularly in environments with deteriorated ambient air quality.

Geographical origin classification of fish using isotopic and elemental signatures with machine learning

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Accurate identification of fish geographical origin is essential for food authentication and traceability. Reliable provenance assessment requires not only robust analytical markers, but also authentic reference datasets that enable meaningful comparison of unknown samples. In this study, stable isotope and elemental data were incorporated into the IsoFoodTrack reference database, and machine-learning approaches were used to evaluate geographical origin of gilthead seabream.

A total of 115 gilthead seabream samples were analysed using a combination of stable isotope ratios ($\delta^{13}C$, $\delta^{15}N$, $\delta^{34}S$, $\delta^{18}O_{water}$) and concentrations of 20 trace and major elements. After excluding samples with missing values, 70 samples were retained and evaluated using a 5-fold stratified split (56 training, 14 testing samples per fold).

We developed classification models to predict geographical origin (Malta, Portugal, and Spain). Two tree-based machine-learning approaches, Decision Tree (DT) and Random Forest (RF), were selected due to their interpretability and strong performance on structured data. Models were trained under consistent conditions across all splits, using isotope and elemental data as predictors.

Results indicate that isotopic and elemental signatures provide strong discriminatory power, reflecting stable environmental and dietary conditions characteristic of production sites. For geographical origin prediction, Random Forest achieved the highest accuracy (97.0% ± 5.7), outperforming Decision Tree (92.8% ± 4.5). These findings confirm the effectiveness of chemical fingerprinting combined with machine learning for seafood authentication.

Finally, the obtained results will be compared with standard statistical methods to further validate model performance.

Identifying the sources of dark brown carbon in the Ljubljana region

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The complex and diverse atmospheric organic aerosols have an immense influence on air quality, human health, and climate. Among these, dark brown carbon (d-BrC) is a recently recognized fraction of brown carbon (BrC) that is water-insoluble, thermally stable, atmospherically persistent, and absorbs light in the visible to near-infrared spectral regions. Despite lower absorptivity than black carbon (BC), d-BrC can represent a substantial fraction of biomass-burning aerosol [1]. In addition to biomass burning, recent studies suggest that fossil fuel combustion may also contribute to d-BrC [2]. However, other sources of d-BrC, as well as its chemical structure and properties, remain poorly understood. Our research aims to detect d-BrC compounds in atmospheric particles and to define d-BrC sources through a source apportionment study. To achieve this, we analysed different tracers in particulate matter collected on quartz fiber filters in Ljubljana using ion chromatography (IC) for water-soluble ions, gas chromatography-mass spectrometry (GC-MS) for levoglucosan and polycyclic aromatic hydrocarbons (PAHs), UV-Vis spectroscopy for optical properties, and inductively coupled plasma mass spectrometry (ICP-MS) for soluble metals. In addition, particle number concentration and size distribution were measured using a scanning mobility particle sizer (SMPS).

We observed enhanced absorption in the near-IR region relative to blanks, indicating the presence of d-BrC compounds. By integrating these measurements with multivariate statistical analysis, this work will constrain d-BrC sources in the Ljubljana region and provide new insight into a poorly understood but atmospherically relevant class of light-absorbing organic compounds.

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Development of a 3D in vitro liver model for genotoxicity testing

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The increasing number of environmental and pharmaceutical xenobiotics to which humans are exposed makes reliable genotoxicity testing more important than ever. The need to reduce animal use under the 3R principles reinforces the demand for advanced, human-relevant *in vitro* systems that can accurately predict human genotoxic responses. Classical 2D liver cell models lack physiological architecture and show reduced CYP450 activity, whereas 3D models from hepatocellular carcinoma lines improve metabolism but still fail to reproduce key hepatic features such as normal karyotype, mature phenotype, and proper DNA repair mechanisms. Recent advances in stem cell biology have enabled the generation of hepatic organoids derived from human induced pluripotent stem cells (hiPSCs), offering unprecedented physiological relevance.

The aim is to develop a 3D liver organoid model derived from hiPSCs, with high physiological relevance, functional liver characteristics, and metabolic capacity. Liver organoids will be expanded in a dynamic bioreactor to mimic optimal physiological conditions and enhance maturation, metabolic competence, and generate high numbers of uniform organoids. Their suitability for genotoxicity testing will be assessed.

The methods summarize the directed differentiation of hiPSCs from pluripotency to endodermal lineage specification, followed by hepatic specification and maturation, verified via transcriptional, proteomic, and functional assays. Liver organoid functionality is confirmed through albumin secretion, urea production, glycogen and lipid storage, and CYP450 enzyme activity. Genotoxicity suitability will be assessed using comet and micronucleus assays, complemented by mechanistic biomarkers of DNA damage and genome instability.

In conclusion, this work aims to establish a next-generation, human liver model for xenobiotic genotoxicity testing, bridging a critical gap between advanced liver biology and genetic toxicology.

Variable sinking speed modelling of gelatinous zooplankton

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Gelatinous zooplankton (GZ) may play an important role in the ocean's biological carbon pump by feeding on smaller planktonic organisms or by transporting particulate organic carbon (POC) to the deep ocean. However, estimates of this vertical transport efficiency vary greatly between studies and are difficult to verify due to experimental limitations. Here, modeling can help identify the most sensitive parameters in the processes involved. Recently, we derived a variable vertical sinking speed model from Newton's second law, which we coupled to the GZ mass [1]. There, we showed that previous estimates of GZ-derived POC export to the seafloor (1.20 Pg C y^{-1}) were overestimated by 14% globally when accounting for deceleration as the particles decay [1]. The largest differences occurred in warmer oceans, where the feedback between sinking speed and GZ decay was enhanced.

Here, we present some key findings from Ref. [1] and discuss the study's limitations. Namely, that GZ were not explicitly included in biogeochemical models and failed to account for any feedback that their presence may exert on other organisms (e.g., [2]). We thus explore ways of incorporating a GZ variable sinking speed model into biogeochemical models. Accurate representation of GZ within the ocean ecosystems will help close the oceanic carbon budget and thus improve our understanding of the processes affecting the global climate.

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Electrochemical impedance spectroscopy for measuring surfactant-induced surface tension changes at a mercury electrode

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Atmospheric aerosol particles are fine particles suspended in the air that influence atmospheric processes and global climate. A significant part of aerosol particles' composition consists of surface-active substances (SAS), amphiphilic compounds containing hydrophobic and hydrophilic groups that partition at the gas–liquid interface and reduce surface tension. This reduction can affect particle formation, growth, size distribution, optical properties, and cloud condensation nuclei activation [1].

Recently, we introduced an electrochemical methodology based on alternating current voltammetry capable of detecting SAS-induced changes in interfacial surface tension at concentrations below the sensitivity limits of conventional tensiometric techniques commonly used in atmospheric sciences [2].

Building on this work, the present study focuses on optimizing the method for quantifying surface-tension changes at a mercury electrode using electrochemical impedance spectroscopy. The approach is based on measuring variations in the double-layer capacitance at the electrode–electrolyte interface, which are influenced by SAS adsorption. From the capacitance data, the surface charge can be determined and related to surface tension via the electrocapillary equation. Optimization of parameters (potential, electrolyte concentration, accumulation time) enabled sensitive detection of SAS.

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Isolation and aggregation of bacteria capable of reducing hexavalent chromium

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Hexavalent chromium (Cr(VI)) compounds are toxic and carcinogenic. Numerous studies have investigated the use of microorganisms to reduce Cr(VI) to its trivalent form (Cr(III)), which is considered significantly less toxic [1]. In this study, the microorganisms were isolated from soil containing elevated Cr concentrations, present as Cr(III). The bacteria were coated with polyethyleneimine to promote the formation of bacterial aggregates. These aggregates were stabilized in alginate beads prior to inoculation onto the culture media. Instead of the nutrient-rich media, the cellobiose was used as a carbon source for bacterial growth, and known concentrations of Cr(VI) were used as a limiting factor (Figure 1). The aggregates were selected based on their growth and doubling time in such conditions. To evaluate the extent of reduction, Cr(VI) concentrations were determined at time points from 1 to 7 days with a diphenylcarbazide assay consisting of 1% 1,5 diphenylcarbazide in absolute ethanol and 0.5 M sulfuric acid. Absorbance was measured in microplates at 540 nm with a BioTek Synergy H4 Multi-Mode Microplate Reader. The method requires further validation.

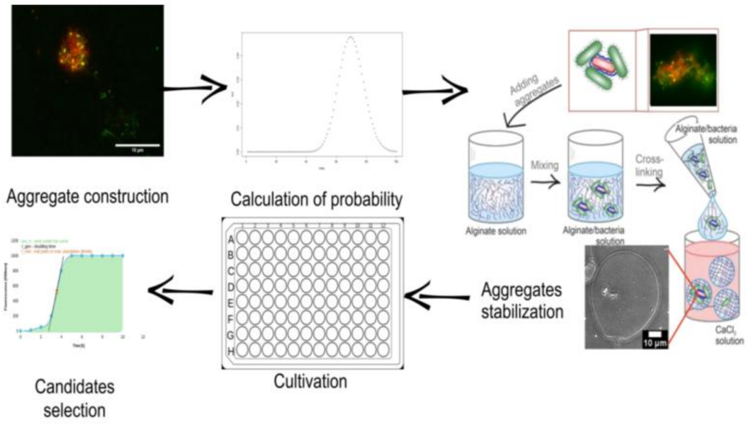

Figure 1. Schematic workflow of the preparation and selection of bacterial aggregates.

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MAP-Bio: A new paradigm for biofilm analysis by massively arrayed particle biofilms

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Bacterial biofilms represent the dominant microbial lifestyle, exhibiting diverse metabolic capabilities and increased resistance to compounds that affect biofilm formation and stability. Assessing their formation, growth dynamics, and disruption remains challenging due to high heterogeneity and stage-dependent development. Conventional methods are often low-throughput, subjective, and require separate assays for planktonic growth, surface attachment, and maturation, providing only a simplified view of the overall system. To bridge this gap, we introduce MAP-Bio: a particle-based flow cytometric platform that fundamentally shifts the focus from observing isolated biofilms to analyzing entire microbial systems in suspension. Using solid particles and strategic staining, MAP-bio tracks cell proliferation, viability, and system dynamics with high statistical power, allowing for a comprehensive assessment of the system in a single run. Capturing the interplay between planktonic and surface-attached states beyond the capabilities of conventional methods. The effectiveness of the method was validated by quantifying biofilm formation across different media and evaluating a novel antimicrobial compound to determine its specific mechanism of action. Flow cytometry differentiated planktonic and surface-attached cells, while SYTO 13 and Live/Dead staining allowed tracking of biofilm formation and maturation dynamics. The results demonstrate that the method can differentiate between unstressed systems and those exposed to the compound. Specifically, the platform successfully assessed system dynamics and identified the stages of biofilm formation most affected by inhibition. MAP-Bio establishes a rapid, objective, and statistically robust framework for real-time monitoring of biofilm formation and its responses to compounds, media conditions, and other parameters. This framework opens new possibilities to study and identify developmental stages most susceptible to inhibition, thereby advancing understanding of microbial ecosystems and enabling investigation of antimicrobial mechanisms of action.

High-resolution anthropogenic benzo[a]pyrene emission inventory for Slovenia for chemistry transport modelling

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Benzo[a]pyrene (B[a]P) is a toxic organic compound with carcinogenic, mutagenic, and teratogenic effects on human health, emitted mainly from the incomplete combustion of fossil fuels and biofuels. It is widely monitored under international frameworks such as the UNECE Convention on Long-Range Transboundary Air Pollution (CLRTAP) and, according to Directive (EU) 2024/2881/EC, used as a marker for total exposure to carcinogenic polycyclic aromatic hydrocarbons (PAHs). Chemistry transport models (CTMs) are increasingly applied to assess the spatial patterns and source attribution of B[a]P pollution, but their performance is strongly limited by the spatial resolution and detail of emission inventories. Existing inventories for Slovenia provide limited spatial resolution (0.1°, or approximately 10 km), which is adequate for regional studies but insufficient for country-scale assessments.

This study develops an approach for compiling a high-resolution (0.01°, or approximately 1 km) emission inventory for B[a]P in Slovenia. A top-down method is applied, where national emission totals reported to CLRTP are spatially disaggregated using proxy datasets, including population density, cadastral data, and land cover. The methodology follows the EMEP/EEA Air Pollutant Emission Inventory Guidebook (2023).

The high-resolution inventory significantly improves the representation of spatial emission patterns compared to coarser datasets. It enables better identification of emission hotspots, particularly in urban areas and regions with intensive residential combustion, and provides a more detailed spatial basis for subsequent CTM-based air quality assessments.

High-resolution emission inventories are essential for reliable model assessment of PAH pollution. The proposed approach provides a practical framework for generating refined emission inputs, supporting improved exposure assessment and policy applications. It can also be extended to other PAH compounds with available national totals, enabling consistent high-resolution modeling of PAH pollution.

Mesoporosity modulations in carbon monoliths for enhanced adsorption of pharmaceutical contaminants

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The occurrence of pharmaceutical active compounds (PhACs) in aquatic environments poses a significant environmental and public health concern. The primary source of these compounds is wastewater treatment plant effluents, as conventional wastewater treatment processes are not designed to remove them effectively. Advanced adsorption materials such as carbon monoliths (CMs) have emerged as promising candidates for quaternary treatment, a final polishing step designed to remove micropollutants. However, controlling their hierarchical porosity, which is key to improving their efficiency, remains a challenge due to phase separation during synthesis. This study aimed to develop high–surface–area hierarchical porous carbon monoliths with tunable mesoporosity using a soft-templating sol–gel approach. Pluronic block copolymers were applied at varying concentrations and in combined formulations to tailor the pore structure. The resulting materials were evaluated for the adsorption of metronidazole (an antibiotic) and paroxetine (an antidepressant). Results show that mesopore size and volume are primarily governed by the formation of Pluronic micelles during polymerization, while microporosity remains comparable across all samples. Also, a strong correlation exists between mesoporous structure and performance, with maximum adsorption capacities reaching 130 μmol g^{-1} for paroxetine and 112 μmol g^{-1} for metronidazole. Enhanced mesoporosity significantly improved mass-transfer kinetics and adsorption efficiency, demonstrating high removal efficiencies (>94–98%) for both compounds. This suggests a strong affinity of the target compounds for the adsorbent surface. Laboratory-scale experiments were conducted in deionized water; therefore, further studies using real wastewater matrices are needed to validate the removal performance of this promising material under realistic conditions.

Every oil has a unique signature

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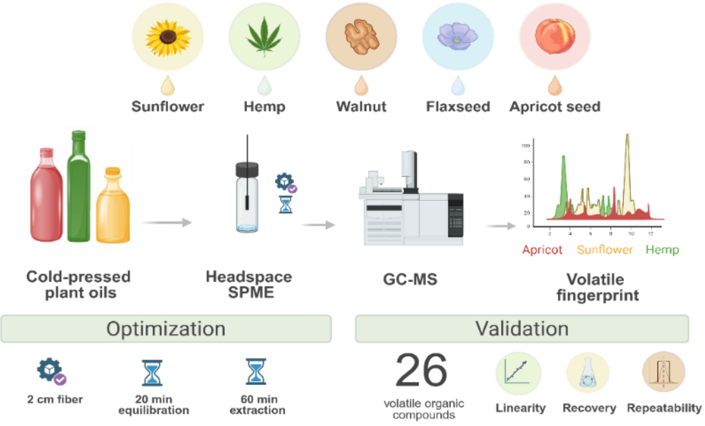

Figure 1. Graphic abstract

Cold-pressed plant oils are gaining attention due to their beneficial effects on human health and their rich natural composition. Because they undergo minimal processing, these oils retain many naturally occurring volatile compounds that contribute to their characteristic aroma and overall quality. In Slovenia, many small-scale producers produce cold-pressed oils from various plants. Therefore, developing a method that provides greater insight into their volatile composition and potential biomarkers, which helps protect authenticity, is essential.

Headspace solid-phase microextraction coupled with gas chromatography–mass spectrometry (HS-SPME GC-MS) is a sensitive technique capable of profiling the volatile compounds of each oil. In this study, we developed the first step of an analytical approach for characterizing volatile compounds in cold-pressed oils.

Extraction conditions were optimized by evaluating fiber length, equilibration time, and extraction time. The optimal parameters were determined to be a 2 cm fiber, 20 min equilibration, and 60 min extraction, providing efficient recovery of compounds with different physicochemical properties.

The method was validated using 26 representative volatile compounds spanning different chemical groups, including alcohols, aldehydes, carboxylic acids, esters, ethers, ketones and terpenes. Validation included assessment of linearity, accuracy, limits of detection and quantification, and matrix effects.

Finally, the optimized method was applied to 13 authentic cold-pressed oils, confirming its applicability to diverse oil types and highlighting distinct volatile profiles among samples. This work represents an important first step toward comprehensive characterization of cold-pressed oils. Future research will combine volatile profiling with sensory evaluation and isotope ratio analysis to further investigate oil authenticity and botanical origin.

Information and Communication Technologies

Predicting electrical power in a grinding process

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Efficient energy management is becoming increasingly important in industrial manufacturing due to rising energy costs and the transition toward low-carbon production systems. Accurate short-term forecasting of electricity demand enables manufacturers to optimize production schedules, stabilize process parameters, and reduce operational costs. This study investigates the prediction of electrical power consumption in an industrial grinding process using machine learning models and historical production data.

The research uses industrial process data collected between 2022 and 2025. The dataset includes operational variables such as grinding speed, dosing speed, specific electrical consumption, and anonymized material properties, complemented by environmental variables. Because the raw data originated from sensors with different sampling frequencies, it was resampled to a uniform one-minute resolution and cleaned to remove startup phases and anomalies. Extensive feature engineering was applied, including rolling statistics over 90-minute windows and long-term weather aggregates over three weeks to capture process dynamics and environmental influences. Several regression models were evaluated, including regularized linear models and tree-based ensemble methods, under different operational scenarios reflecting the availability of planned process setpoints.

The results indicate that regularized linear models, particularly Ridge Regression, provided the most reliable and stable predictions. When planned operational setpoints were included, the model accurately forecasted electrical power demand up to 30 minutes ahead while maintaining strong performance across longer prediction horizons.

These findings demonstrate that carefully engineered features combined with interpretable machine learning models can provide accurate short-term energy forecasts in industrial processes. Such predictive capabilities can support proactive energy management strategies, enabling manufacturers to stabilize production, improve efficiency, and reduce energy-related costs and emissions.

Acknowledgments: The research has received funding from the Slovenian Research Agency grant P2-0001 and from DIGITOP, GA no. TN-06-0106, funded by the Ministry of Higher Education, Science and Innovation of Slovenia, Slovenian Research and Innovation Agency, and European Union - NextGenerationEU.

Swarmalators: the connection between synchronization and collective motion

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Synchronization and collective motion are two manifestations of self-organization in complex systems, appearing in contexts ranging from neural activity and cardiac dynamics to animal swarms and coordinated robotic systems. Traditionally, these phenomena have been studied separately: synchronization concerns the alignment of internal oscillatory phases, while collective motion describes the emergence of ordered spatial patterns through local interactions. Recent theoretical developments combine both aspects in a unified framework known as swarmalators [1]. Here, we present the basic swarmalator model and its main dynamical properties. We introduce the mathematical formulation of the model and explain the role of its key parameters and coupling terms that link spatial motion with phase synchronization. Numerical simulations and qualitative analysis illustrate the emergence of characteristic collective states, including synchronized clusters, phase waves, and mixed spatial–phase patterns (Figure 3). These regimes can be systematically distinguished using order parameters that quantify spatial organization and phase coherence. The results show that bidirectional coupling between phase synchronization and spatial motion produces collective behaviors that cannot be captured by models of synchronization or collective motion alone [2,3]. In addition to presenting the Kuramoto-type phase dynamics used in the basic model, we will outline in this contribution directions for further research, particularly the extension to alternative synchronization mechanisms such as the excitable theta-neuron model.

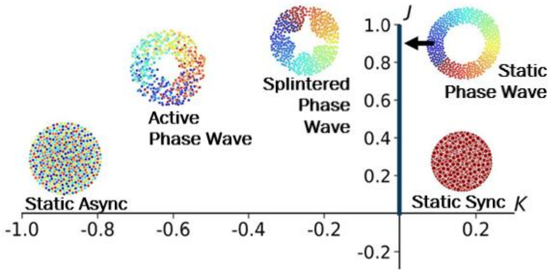

Figure 3: Dynamic patterns of swarmalators for different values of the coupling parameter between phase and spatial motion *J* and the phase coupling parameter *K*, adapted from [2] and [3].

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Large language models for word sense disambiguation

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Word sense disambiguation (WSD) is a critical step in natural language processing (NLP), referring to the process of determining the correct meaning (sense) of an ambiguous word. In biomedical literature analysis, WSD is needed for accurate interpretation of ambiguous abbreviations and symbols, for example, the symbol "AA" can refer to "Amino Acids" or "Alcoholics Anonymous" depending on the context. Traditional WSD approaches rely heavily on manually annotated training corpora, limiting their scalability across biomedical subdomains. In this work, we propose the use of large language models (LLMs) as scalable, zero-shot classifiers for disambiguating biomedical abbreviations and symbols in the MeSH Word Sense Disambiguation dataset (MSH-WSD). MSH-WSD is a standard benchmark dataset, featuring 203 ambiguous abbreviations, symbols, and terms sourced from the MEDLINE database. LLM-based WSD was conducted using Gemma 3:27B and MedGemma 27B and compared against XGBoost, a symbolic learner based on decision tree ensembles. XGBoost was trained using term frequency-inverse document frequency features extracted from labeled examples, with a 2/3 train and 1/3 test split per symbol. The proposed LLM-based approach using MedGemma reaching 0.92 precision and 0.88 recall, Gemma 3 achieving 0.91 and 0.89, respectively, yielded results comparable to those of XGBoost that achieved 0.94 on both metrics. The higher precision relative to recall observed in the LLM models suggests that while they occasionally fail to identify the correct sense, the models demonstrate high precision when a prediction is made. The principal advantage of the proposed LLM-based approach lies in its applicability: it produces competitive predictive performance without requiring any manually annotated training data, eliminating the data preparation step required by supervised approaches. This has significant applicative value, as such zero-shot disambiguation may substantially facilitate the reimplementation of NLP tools in the biomedical domain.

A new multi-objective optimization algorithm using the covariance matrix adaptation evolution strategy

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Multi-objective optimization of black-box problems requires algorithms capable of efficiently navigating complex, hard-to-solve landscapes. The Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [1] is a highly effective single-objective optimizer, and several approaches (such as MO-CMA-ES [2], HMO-CMA-ES [3], and COMO-CMA-ES [4]) have adapted it for multi-objective problems. To further improve efficiency, we propose a novel CMA-ES-based multi-objective approach, which launches CMA-ES kernels one by one, uses different search tactics depending on the current state of the algorithm and keeps a global archive of all evaluated solutions. We use the global archive to determine the next scalarized objective to be optimized and compute from it the local landscape data, which is then used for an informed CMA-ES kernel initialization. We also introduce a dedicated front refinement phase for the later stages of the algorithm. This phase uses the global archive to estimate good sampling distributions to fill in the regions between the points of the algorithm's empirical front. Preliminary evaluations on multi-objective benchmark problems show encouraging results in terms of overall efficiency. Ultimately, this unconstrained approach serves as a stepping stone toward adapting the algorithm for constrained multi-objective optimization, which is not covered by existing multi-objective CMA-ES variants.

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Towards Expert Local AI: Boosting Open-Weight Language Model Performance in Material Science

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Open-weight large language models (LLMs) perform well in domains with abundant open-access data, such as Computer Science and Mathematics. However, they struggle with Natural Sciences like Material Science (MS) due to the lack of high-quality MS datasets, as the literature is typically paywalled and stored in proprietary formats, creating a severe training data bottleneck [1]. Consequently, a significant knowledge gap exists between well-funded proprietary LLMs with access to proprietary content and open-weight models, as well as concerns regarding ethics [1]. While some small, domain-specific open-weight LLMs, such as MedGemma [2] exist, their performance is dependent on the data availability. Our research aims to bridge this gap by improving open-weight LLMs' ability to understand and answer domain-specific MS questions. To overcome data scarcity, this study leveraged institutional Text and Data Mining (TDM) access via Elsevier's APIs to retrieve a corpus of full-text MS publications from 1996 to 2021. We employed the Gemini 3 Pro model to perform synthetic data transformation. For each retrieved article, the model was prompted to generate 10 distinct question-answer pairs (open-ended, numerical, and multiple-choice) based on the paper's methodology and results. This approach resulted in an instruction-tuning dataset comprising 635,245 pairs suitable for instruction-tuning open-source LLMs in the MS domain.

We established a performance baseline using the open-weight Gemma-3-4B model [3] evaluated on the MaScQA benchmark [4]. For a preliminary feasibility test, we employed a dynamic few-shot prompting strategy, where for each MaScQA benchmark question, 5 most semantically similar question-answer pairs were provided as in-context examples to the model. This increased the model's accuracy on MaScQA from 26.8% to 35.4%. This initial 8.6% improvement demonstrates that open-weight models can successfully utilize MS data, yet the low 35.4% peak indicates significant room for growth. Building on these findings, ongoing work focuses on instruction-tuning Gemma-3-4B to further enhance its domain understanding.

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Exact equation discovery from implicit, rational, and polynomial data

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Equation discovery aims to recover mathematical relationships directly from data, making it a promising tool for scientific research across many fields, from physics and chemistry, to molecular biology and biotechnology, materials science, and environmental sciences, including isotope tracing. While most current methods aim to recover approximate equations from noisy measurements, we focus on exact equation discovery, where the objective is to identify equations that describe noise-free data perfectly.

Integer sequences provide a natural benchmark for this task. For instance, from the Fibonacci sequence (0, 1, 1, 2, 3, 5, 8, . . .), one can ask whether an algorithm can recover the recurrence ($a_n = a_{n-1} + a_{n-2}$). In earlier work, we evaluated methods based on Diophantine equation solving and Gröbner basis computation on explicit equations arising from OEIS sequences, including some non-linear examples. However, only linear equations were studied at scale. In this study, we extend that setting to more general classes of equations.

We constructed a benchmark of datasets generated from 20 implicit equations, 129 rational equations, and 2,257 polynomial equations, and used it to compare our methods with state-of-the-art approaches. The results show a clear pattern: Gröbner basis methods remain the only viable option for implicit and rational equations, whereas polynomial equations are handled significantly better by Diophantine-equation-based methods. The main drawback of the latter is high computational complexity. These findings show that exact equation discovery benefits from combining ideas from machine learning, symbolic computation, and algebra, and that different equation classes require different computational tools.

Bi-objective Heterogeneous Green Vehicle Routing: Preliminary Investigation Using Weighted-Sum Scalarization and PyVRP

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The Capacitated Vehicle Routing Problem (CVRP) is a classical optimization problem that seeks to determine efficient delivery routes for a fleet of vehicles with limited capacity, typically formulated as a single-objective problem that assumes a homogeneous fleet and distance-based cost minimization. In recent years, attention to the environmental impact of transportation has motivated the development of multi-objective routing models. In this work, we investigate a CVRP extension with a heterogeneous fleet of conventional diesel and low-emission vehicles. We formulate this as a bi-objective optimization problem with two objectives: minimizing total travel distance and total CO_2 emissions, while ensuring capacity feasible routes. The two vehicle types differ in capacity, fleet size, and emission rates. Emissions are modeled using a load-dependent function following the Pollution Routing Problem [1]. As a preliminary approach, we employ a weighted-sum scalarization that converts the bi-objective problem into multiple single-objective instances with varying preference weights. These are solved using PyVRP, a hybrid genetic algorithm solver for vehicle routing problems [3]. Computational experiments on adapted X benchmark CVRP instances [2] approximate the Pareto front and demonstrate the trade-offs between total travel distance and CO_2 emissions, relevant to sustainable transportation planning worldwide.

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Data driven approaches to nanoparticle protein corona formation

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When vaccines or other nanoparticles enter biological environments such as the human body, their surface becomes coated with proteins and biomolecules, which can change their biological identity and functionality. A Protein corona is a protein-rich layer that forms around nanoparticles that may affect their performance and safety in nanobiomedical applications. However, identifying or predicting protein corona formation is quite challenging because it depends on multiple physicochemical and experimental factors, including nanoparticle charge and size, as well as the corona isolation method. In this study, we applied machine learning and data analysis tools to address these challenges. Our approach leverages predictive and descriptive machine learning and data analysis techniques to predict protein corona formation. We apply these techniques to a dataset containing physicochemical properties of nanoparticles, nanoparticle characteristic techniques, and properties of the biological source. Our results show that a combined machine learning and data analysis approach to protein corona prediction can not only support systematic protein corona analysis by guiding nanomaterial design and safety, but also help uncover hidden patterns in protein corona formation that were not identified before.

Enabling physically feasible manipulation of extended tools through redundancy-driven interaction

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Robotic manipulation with extended tools introduces significant physical challenges that are not captured by kinematic planning alone. When forces are applied at a distance, the resulting lever-arm effect increases joint torques and can make otherwise feasible tasks difficult or impossible to execute. This limitation is particularly relevant in applications such as painting, cleaning, or inspection, where long tools are commonly used.

In our research, we investigate control strategies that explicitly account for these physical effects. The proposed approach exploits kinematic redundancy to introduce secondary objectives in the null space of the controller, allowing the robot to adapt its configuration while maintaining the primary task defined at the tool endpoint. We consider methods based on minimizing externally induced joint torques as well as interaction forces measured at the robot flange.

An important aspect of the approach is that it does not rely on explicit modeling of the environment. Instead, the robot adapts its posture based on force feedback, which can lead to the emergence of supportive contacts that help redistribute loads. The method is evaluated on a 7-DOF manipulator equipped with a long tool in a set of static, dynamic, and contact-rich tasks.

The results show that redundancy can be used to improve load distribution while preserving task execution. The robot is able to maintain stable motion and force control under varying conditions, while reducing the effect of external loading. This suggests that incorporating interaction-aware objectives into redundancy resolution can improve the feasibility of extended-tool manipulation and provides a basis for further investigation, including potential extensions to cooperative multi-robot systems.

The Impact of Document Splitting on Question-Answering Systems Quality

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Modern language models often need to retrieve external knowledge to answer questions accurately. How a system splits documents into searchable segments — a process known as chunking — directly determines what information the model can find. Most systems use fixed-size or sentence-based splitting, ignoring the natural structure of documents. This can fragment technical content and weaken retrieval quality, particularly across languages.

To address this, we introduce a structure-aware chunking method that preserves meaningful boundaries in multilingual technical documents, such as headings, tables and hierarchical sections. We evaluated the approach on a bilingual English–Slovene corpus across three retrieval methods: keyword matching (TF-IDF), statistical ranking (BM25), and neural semantic search (Sentence Transformers). Structure-aware chunking improved retrieval accuracy by up to 32% with the neural model and achieved near-equal performance across both languages, while BM25 showed the most stability across chunk strategy and language.

However, modern question-answering systems go beyond simple retrieval. Agentic architectures use a reasoning loop where the system decides how to search, whether to reformulate its query and when it has enough context to respond. It remains an open question whether retrieval-level improvements from better chunking, translate into better reasoning behavior from the agents.

In this work, we extend our evaluation to an agentic pipeline built around a ReAct (Reasoning + Acting) reasoning agent. We present the system architecture and describe our experimental plan for analyzing agent behavior under different chunking conditions. We measure the number of reasoning steps per query, query reformulation frequency, answer refusal rates on answerable questions, and per-language division in these patterns. The goal is to determine whether chunking, which is typically treated as a retrieval concern, meaningfully shapes the downstream reasoning process in multilingual question-answering systems.

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Computational graphs for parameter estimation in symbolic regression

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Symbolic regression, or equation discovery, aims to identify a closed-form mathematical equation that best describes observed data. The process typically consists of two stages. First, a candidate equation structure is generated, often containing unknown constants treated as free parameters. Second, these parameters' values are estimated from the data, usually using numerical optimization. In this work, we investigate computational graphs as an alternative approach for parameter estimation.

A computational graph is a directed graph representation of a mathematical expression that enables efficient evaluation. During the forward pass, values for variables and constants are provided at the input, and the value of the expression is obtained at the output. A loss function then measures the discrepancy between the predicted and target values. During the backward pass, automatic differentiation computes the gradients of the loss with respect to the constants. Treating these constants as learnable parameters allows their values to be optimized through backpropagation using a gradient-based optimization algorithm.

We perform parameter estimation on all 66 equations containing constants from the "Feynman Lectures on Physics" [1]. The performance of computational graphs is compared with three classical optimization methods and four machine learning-based methods. Our results show that computational graphs achieve performance comparable to traditional optimization methods and outperform the machine learning approaches. However, they are also the most computationally demanding and, similarly to optimization methods, can produce invalid estimation attempts. Under noisy conditions, machine learning methods slightly outperform both optimization methods and computational graphs.

Overall, our findings indicate that computational graphs are a competitive alternative for parameter estimation, particularly when working with exact data. In contrast, machine learning-based approaches appear more robust in noisy settings. Future work will focus on integrating these methods into a complete equation discovery pipeline to better assess their practical advantages and limitations in real-world symbolic regression tasks.

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Capability-guided execution for robust dual-arm robot cloth unfolding

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Robot cloth unfolding is a fundamental primitive for cloth manipulation and a prerequisite for most downstream tasks. In the regrasping-in-the-air approach, benchmarked at the ICRA 2024 Cloth Competition, one arm holds the cloth in a hanging state while the other executes a learned 6-DoF grasp to maximize visible cloth coverage after stretching. In our previous work, we reproduced this pipeline on a dual-arm robot cell using the CeDiRNet-6DoF grasp predictor, achieving 59% average coverage and 68% grasp success. These results show that learned perception generates viable candidates, but execution remains a bottleneck: inverse-kinematics failures, joint-limit and collision constraints, and low task-direction dexterity, especially near singularities, render many predicted grasps non-executable. This is further amplified by dual-arm coupling, since the holding arm configuration affects the reachable and collision-free workspace of the grasping arm. A simple heuristic that repositioned the cloth when grasps were infeasible reduced the unattempted grasp rate by 6.7pp over 1360 trials, confirming that even simple cloth repositioning improves execution reliability.

Our current work replaces this heuristic with a principled capability-guided execution layer that keeps the grasp predictor unchanged. Offline, we compute capability maps for the 7-DoF grasping arm by sampling joint space, evaluating forward kinematics and storing per-voxel scores that combine reachability, joint-limit margin, manipulability and directional manipulability along the grasp approach vector - thereby capturing task-relevant dexterity beyond the classical manipulability index. Online, the system queries the map for each predicted grasp and, if the score is low, determines a repositioning target for the holding arm that shifts the grasp into a higher-capability workspace region.

We evaluate the approach by comparing grasp feasibility and coverage with and without capability-guided repositioning. The expected outcome is fewer planning failures, higher grasp success and improved end-to-end reliability and coverage, addressing a practical gap between learned grasp prediction and robot-specific execution.

Graph instance landscapes: when structural similarity does (not) reflect shortest-path performance

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Benchmarking shortest-path algorithms usually reports aggregate results over heterogeneous graph sets, giving limited insight into how runtime behavior relates to graph structure. We adopt an instance-landscape perspective in which graphs are embedded in a low-cost structural feature space, clustered into regions of similar structure, and then analyzed with respect to structural and performance similarity.

Three benchmark suites are considered: weighted Erdos-Renyi graphs, random geometric graphs, and real-world road networks. Each instance is described by 17 structural features, including density, degree statistics, and edge-weight characteristics. Landscape regions are identified by k-means clustering with silhouette-based model selection. Four representative shortest-path algorithms are evaluated: Dijkstra, bidirectional Dijkstra, A*, and a deque-based strategy (DEQ). Runtime distributions across regions are compared using Anderson-Darling and Kolmogorov-Smirnov tests.

Generator parameters induce stable and well-separated structural regions: edge density dominates random graphs, while connection radius organizes geometric graphs. Road networks occupy distinct areas from synthetic benchmarks in a merged-suite t-SNE view. However, structural proximity does not guarantee performance equivalence. Significant runtime shifts are often observed even within the same structural region, especially for Dijkstra, bidirectional Dijkstra, and DEQ, whereas A* is more robust but not invariant.

These results show both the value and the limits of feature-space landscapes for structure-aware benchmarking and shortest-path algorithm selection.

Recipe Similarity Evaluation with Multi-View Metrics and Large Language Model Judges

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We present a redesigned evaluation framework for recipe similarity estimation that integrates classical engineered metrics with large-scale judgments from multiple Large Language Models (LLMs). Building on prior multi-view similarity methods combining lexical, semantic, and nutritional features, we address key limitations of existing evaluations, including reliance on small expert-labeled datasets, lack of strong baselines, and restricted sampling of the similarity space. We first calibrate similarity thresholds using an expert-agreed dataset of 255 recipe pairs, then construct balanced evaluation sets spanning clearly dissimilar, borderline, and highly similar recipes. Five LLMs are employed as near-gold-standard judges of recipe similarity. We compare single-view baselines and a fused multi-view system against aggregated LLM judgments, analyzing agreement, failure modes, and trade-offs relative to zero-shot LLM recommendations. Our results demonstrate that multi-view fusion consistently aligns more closely with LLM reasoning than any single metric, while engineered similarity retains advantages in stability, efficiency, and interpretability.

Nanotechnologies

TGA/DSC Analysis of Atmospheric and Graphite Development of a drug delivery system inspired by the red blood cell mimicry

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Targeted drug delivery systems are essential to improve the efficacy of cancer treatments while minimizing systemic toxicity. This research focuses on the development of complex biomimetic liposomes inspired by red blood cell mimicry [1], designed to deliver therapeutic agents to cancer cells specifically through receptor-mediated targeting. The project involves the synthesis of liposomes modified with custom-made protein-mimetics, aiming to bridge the gap between nanotechnology and clinical oncology. The liposomes were prepared using the thin-film hydration method followed by extrusion through 200 nm polycarbonate membranes to achieve a uniform size distribution. The lipid formulation included a complex mixture of phospholipids (DSPC, DPPC, DOPC, DOPE, LSPC, SM), cholesterol, and gangliosides, with DSPE-PEG-maleimide incorporated for peptide conjugation. Characterization was performed via Dynamic Light Scattering (DLS), Zeta potential measurements, and Transmission Electron Microscopy (TEM). Recent laboratory activities focused on optimizing peptide conjugation and evaluating biocompatibility. Hemolysis assays confirmed the excellent safety profile of the formulations, with negligible toxicity (<2%) at working concentrations. A comparison between two functionalization strategies revealed that post-extrusion conjugation (Strategy 1) produces a more monodisperse system (PDI 0.18) compared to pre-incorporation (Strategy 2). In the purified fraction (FR5), surface modification was confirmed by a hydrodynamic diameter increase of ~4 nm and a zeta potential shift toward more negative values, from -6.1 mV to -7.8 mV. These results validate the structural stability of the liposomes post-conjugation, laying the groundwork for future siRNA encapsulation studies.

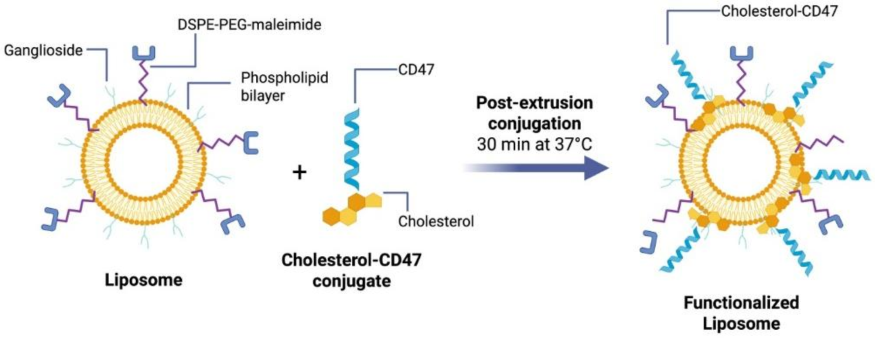

Figure 1. Illustration of the surface modification process for RBC-mimetic liposomes through physical post-insertion of CD47 peptides. Illustration created with BioRender.com.

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Conjugation of neuropeptide Y-analogues to erythrocyte membrane vesicles for active targeting purposes

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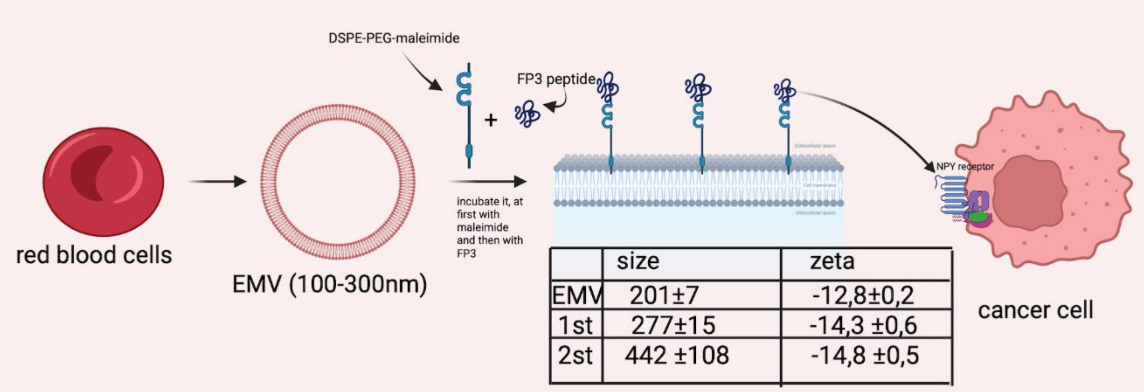
Developing efficient drug delivery systems remains a challenge in oncology. Erythrocytes offer a unique platform for biomimetic carriers due to their *in vivo* biocompatibility and long circulation half-life. This study focuses on functionalizing erythrocyte membrane-derived vesicles (EMVs) with neuropeptide Y (NPY) analogues to achieve active targeting of breast cancer cells. The team isolated EMVs through controlled hemolysis and extrusion to reach a uniform size (100–300 nm). We modified the membrane using DSPE-PEG-maleimide as a linker for the site-specific conjugation of FP3 peptides, acting as NPY-mimetic ligands (Figure 1).

Current results confirm successful membrane isolation and peptide conjugation. Characterization via Dynamic Light Scattering (DLS) and Zeta potential measurements demonstrates the stability and surface charge shifts of the functionalized vesicles. BCA assays further quantify the efficiency of peptide loading while maintaining structural integrity.

In conclusion, these EMV-based carriers combine natural camouflage with high specificity. This approach aims to enhance the therapeutic index of encapsulated drugs. Future work will optimize lipid-to-peptide ratios for clinical applications in breast cancer therapy.



	size	zeta
EMV	201±7	-12,8±0,2
1st	277±15	-14,3 ±0,6
2st	442 ±108	-14,8 ±0,5

Figure 1. Schematic representation of EMV functionalization with FP3 peptide and in vitro characterization.

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Colloidal Stabilisation of Magnetic Nanoplatelets in Low-polarity Solvents

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Ferrofluids (FFs) are stable colloidal dispersions of magnetic nanoparticles in a carrier fluid. Their colloidal stability is governed by the balance between attractive van der Waals interactions driving the agglomeration and the electrostatic and/or steric interactions preventing it. In systems composed of permanently magnetic particles, additional magnetic dipole–dipole interactions arise, promoting agglomeration and making the preparation of stable dispersions even more challenging.

Nevertheless, FFs were prepared from permanently magnetic barium hexaferrite (BHF) nanoplatelets (NPLs) at concentrations sufficiently high to exhibit ferromagnetic ordering [1]. This was done by functionalizing the NPLs with dodecylbenzenesulphonic acid, which induces the formation of an electric double layer that prevents the agglomeration. While ferromagnetic ferrofluids have also been prepared in nonpolar solvents [2], classical electrostatic stabilisation is difficult in media with low dielectric constants, due to the very low degree of ionic dissociation. However, the particle charging in low-polarity solvents has been observed, particularly upon the addition of surfactants [3].

In our work, BHF NPLs were functionalized with ricinoleic acid and dispersed in various non-aqueous solvents to investigate the mechanisms governing colloidal stability in such low-polarity FFs. Chlorinated solvents, including chloroform, dichloromethane and dichlorobenzene, produced the most stable dispersions, exhibiting the highest NPL concentrations and minimal aggregation. While steric and solvation forces arising from interactions between the solvent and the ricinoleic acid tails were initially assumed to dominate the stabilization [2]. Additional analysis revealed measurable zeta potentials in these systems, suggesting that electrostatic repulsion may also contribute to the stability of magnetic NPLs in low-polarity media.

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Magnetism of $Na_3Ni_2BiO_6$ at high pressure and magnetic fields

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High-pressure studies provide a powerful route to tune the crystal structure and magnetic interactions without introducing chemical disorder. Layered nickelate compounds are attractive candidates for such investigations due to their rich phase diagrams under high pressure. One such compound is $Na_3Ni_2BiO_6$, an antiferromagnet (AFM) with a monoclinic α-$NaFeO_2$-type structure in which Ni^{2+} ($S = 1$) ions form two-dimensional honeycomb layers. The compound exhibits long-range AFM order at $T_N \approx 10.4$ K and a positive Curie–Weiss temperature , θ_{CW}, of 13.3 K [1]. In this work, we report systematic investigation of the effect of magnetic field, H, and hydrostatic pressure, p, on the magnetism of polycrystalline $Na_3Ni_2BiO_6$.

At $\mu_0 H = 0.1$ T and $p = 1$ bar, an AFM transition is observed at 10.5 K; a Curie-Weiss fit yields $\mu_{eff} = 3.25\ \mu_B/Ni^{2+}$ and $\theta_{CW} = 13.7$ K in good agreement with the literature [1]. Field-dependent studies demonstrate a systematic suppression of T_N from 10.5 K (0.1 T) to 8.30 K (7 T), as previously reported [2]. Furthermore, we find that hydrostatic pressure further suppresses the AFM ordering. At 0.1 T, increasing p to 1.35 GPa shifts T_N from 10.5 K to 10.2 K ($\Delta T_N/\Delta p = -0.22$ K/GPa), for 5 T the T_N shifts from 9.6 K to 9.0 K ($\Delta T_N/\Delta p = -0.44$ K/GPa) and at 7 T the T_N shifts from 8.9 K to 8.1 K ($\Delta T_N/\Delta p = -0.58$ K/GPa). We tentatively attribute this shift to an anisotropic compression of the layered structure, as observed in the structurally similar compound $Na_3Co_2SbO_6$ [3].

These findings demonstrate that the magnetic ground state of $Na_3Ni_2BiO_6$ is highly tuneable through both pressure and magnetic field. In the future, we plan to investigate single crystals of $Na_3Ni_2BiO_6$ under even higher pressures using diamond anvil cells.

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Modelling oxygen island formation on aluminium surfaces with on-lattice kinetic Monte Carlo

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Kinetic Monte Carlo (kMC) is a computational method capable of highly accurate and efficient simulations of long-timescale processes. In this work, we present the ongoing development of a flexible kinetic Monte Carlo framework, where we move away from validating its functionality with simple toy models to focus on a more realistic example: the earliest stages of aluminum oxidation. As a first step, we consider oxygen adatoms on an aluminum surface and simulate the formation and evolution of oxygen islands as a result of adsorption and diffusion events. The simulations are used to explore how external factors, such as temperature and oxygen partial pressure, affect the morphology of islands formed in the earliest stage of oxidation. The results compared with existing experimental observations and similar computational studies of the system [1]. This work represents a step toward modelling more complex processes involved in aluminum oxidation.

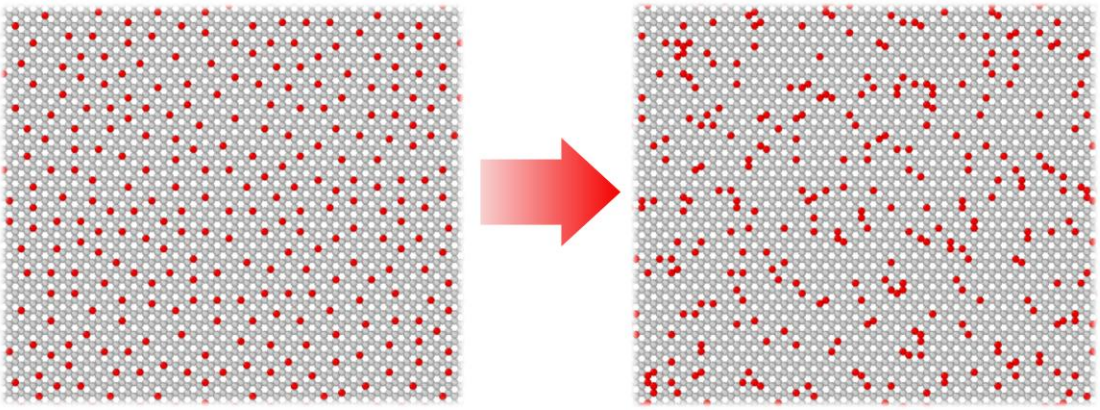

Figure 1. A schematic representation of island formation in a kMC simulation. Occupied sites (adatoms) are shown as red and unoccupied sites as grey. During the simulation the adatoms begin to cluster and form islands, eventually reaching a steady state.

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Ferroelectric thin-film membranes for electrocaloric cooling of wearable devices (FEROCOOL)

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The fabrication of freestanding complex-oxide thin film membranes offers a promising strategy for integrating functional materials into flexible and wearable devices. This approach requires the growth of high-quality sacrificial layers that enable the release of epitaxial films without compromising structural integrity. In the research, we investigated the epitaxial growth of the water-soluble sacrificial layer $Sr_3Al_2O_6$ (SAO) onto $SrTiO_3$ (100) substrates (STO) using pulsed laser deposition. We systematically changed the deposition parameters including substrate temperature, oxygen partial pressure, laser fluence and frequency rate to reduce surface roughness while preserving the single-phase crystalline structure of SAO. Previous studies have through structural and morphological characterization shown cube-on-cube epitaxy of SAO on STO, and that optimized growth conditions yield smooth, phase-pure films suitable for subsequent heteroepitaxial deposition. Minimizing surface roughness prevents defects in functional overlayers and ensures uniform thin film membrane release during the etching process of the sacrificial layer. We also intend to explore Ca-substituted $Sr_{3-x}Ca_xAl_2O_6$ (SCAO) sacrificial layers to tune lattice parameters and dissolution behaviour, which may further improve epitaxial compatibility and membrane release processes [1].

We will use the optimized SAO layers as templates for the growth and release of freestanding ferroelectric and antiferroelectric thin film membranes. In future work, these thin film membranes will include electrocaloric materials such as the relaxor ferroelectric Sm doped $Pb(Mn_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (Sm-PMN–PT) and the antiferroelectric $Pb_{0.8}Ba_{0.2}ZrO_3$, as well as engineered superlattices that combine both systems. Such freestanding structures are expected to enhance thermal management and mechanical compliance, enabling the development of electrocaloric cooling elements for next-generation wearable electronics. Our results establish optimized growth conditions for SAO sacrificial layers and provide a foundation for transferable ceramic oxide heterostructures aimed at flexible solid-state cooling technologies.

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Improving hexaferrite distribution in magnetoactive elastomers

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Magnetoactive elastomers (MAEs) are soft composites of magnetic particles distributed within an elastomer matrix, of which mechanical and surface properties can be tuned in real time using permanent magnets or small electromagnets. This makes them promising candidates for soft actuators and magnetically programmable soft robotic systems; however, their development remains limited by the difficulty of achieving uniform filler distribution within the matrix, as aggregation reduces their performance. We investigated surface modification of strontium hexaferrite fillers with dodecylbenzenesulfonic acid (DBSA) in a polydimethylsiloxane (PDMS) matrix. DBSA adsorption improves chemical compatibility and introduces steric repulsion that counteracts magnetic dipole–dipole and van der Waals interactions responsible for aggregation. DBSA modification combined with freeze-drying substantially improved filler distribution (Figure 1), reducing particle clusters sizes from ~500 µm to ~100 µm as confirmed by micro-CT. This improvement was corroborated magnetically, with a smooth hysteresis loop, consistent with uniform filler distribution. These results demonstrate that controlling filler–matrix interfacial compatibility is a key strategy for improving microstructure and magnetic performance in MAEs.

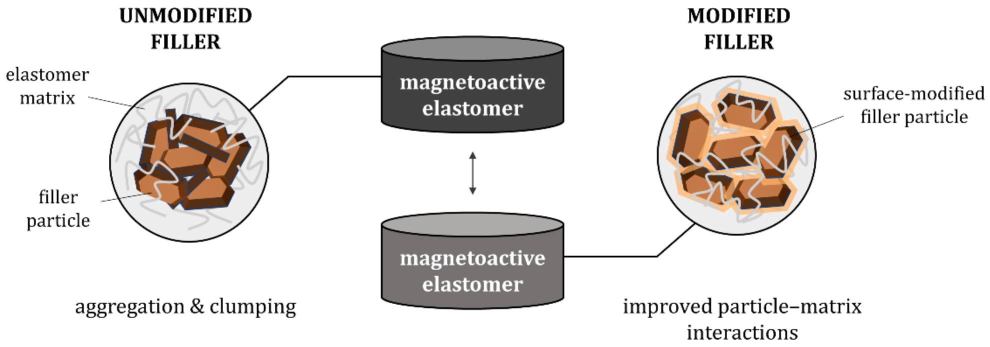

Figure 4. Graphical abstract comparing hexaferrite fillers dispersion in magnetoactive elastomers: left, unmodified filler showing aggregation; right, DBSA-modified, freeze-dried filler with improved dispersion.

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Hydrogen bond pathways for magnetic exchange in mononuclear copper(II) complexes

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Copper(II) complexes display diverse magnetic behaviour due to their d^9 electronic configuration and spin–spin interactions, which may occur even in systems with isolated metal centres as a result of intermolecular contacts such as halide–halide interactions, copper–halide contacts, and hydrogen bonds [1], [2]. We synthesised and structurally characterised six new copper(II) bromide complexes with 1,4-diazabicyclo[2.2.2]octane (Dabco) as ligand. Examination of their magnetic properties showed that magnetic interactions between mononuclear copper(II) centres depend strongly on the nature of the intermolecular exchange pathways rather than on copper–copper separations alone. Complexes lacking N–H-Br hydrogen bonds display only weak antiferromagnetic interactions despite comparable Cu-Cu distances, whereas stronger antiferromagnetic coupling is observed in structures where such hydrogen bonds connect neighbouring complexes (Figure 1). These findings demonstrate that hydrogen bonds and three-dimensional supramolecular connectivity play a crucial role in governing magnetic exchange in mononuclear copper(II) bromide systems.

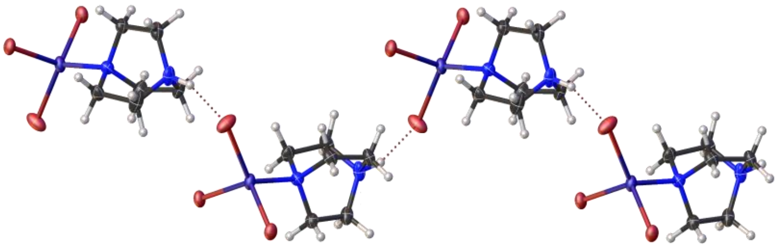

Figure 5. Hydrogen bonds between [HDabco]$CuBr_3$ complexes.

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Artery-specific effects of cGMP on Ca^{2+} signaling: a model-based comparison of pulmonary and mesenteric arteries

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Cyclic 3',5'-guanosine monophosphate (cGMP) is an important regulator of arterial function because it helps control intracellular Ca^{2+} concentration ($[Ca^{2+}]_i$) in vascular smooth muscle cells (SMCs), which determines whether a vessel contracts or relaxes. A decrease in $[Ca^{2+}]_i$ results in smooth muscle relaxation, vessel widening, and lower vascular resistance. Disruption of these signaling pathways may contribute to abnormal vessel constriction and cardiovascular disease. However, the effects of cGMP are not identical across artery types, and the mechanisms behind these differences remain unclear. To investigate this, we developed an extended computational model based on earlier biophysical descriptions of Ca^{2+} signaling [1,2]. The model includes established direct and indirect effects of cGMP and was expanded to account for its influence on Ca^{2+}-activated chloride channels (ClCa). Using this model, we compared SMCs from pulmonary (PA) and mesenteric arteries (MA), which differ in ClCa channel subtype expression [3]. In particular, the MA model includes an additional cGMP-sensitive ClCa subtype that is absent from the PA model. We then simulated responses to increasing cGMP under oscillatory and steady-state conditions and used average $[Ca^{2+}]_i$ as a marker of contractile activity. The simulations showed distinct behaviors in the two artery types. In the PA model, higher cGMP reduced $[Ca^{2+}]_i$, consistent with its expected relaxing effect. However, in the MA model, cGMP above a certain level increased $[Ca^{2+}]_i$, although experimental observations indicate relaxation [3]. This mismatch points to the likely involvement of additional Ca^{2+}-independent regulatory pathways. Our results further indicate that the cGMP-sensitive ClCa channel in MA cells plays an important role in promoting Ca^{2+} entry at high cGMP levels. Overall, the study shows that artery-specific channel composition strongly shapes the cellular response to cGMP and should be considered in models of vascular regulation.

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Bioactive biomaterials based on hydroxyapatite doped with multiple ions for bone tissue regeneration

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Hydroxyapatite (HAp, $Ca_{10}(PO_4)_6(OH)_2$) is the main inorganic component of bone and is widely used in bone tissue engineering due to its biocompatibility and osteoconductivity. However, pure synthetic HAp has limited ability to stimulate bone regeneration actively. Doping with bioactive ions is a promising strategy to enhance its biological performance [1] [2].

In this study, hydroxyapatite doped with multiple ions was synthesized to enhance bioactivity and antimicrobial properties for bone regeneration. The material was simultaneously doped with Sr^{2+}, Mg^{2+}, Zn^{2+}, Ga^{3+}, and Si^{4+} ions, which influence different stages of bone remodeling. Non-doped (HAp), single-doped (HApSi), and multi-doped (HApSrMgZnGaSi) hydroxyapatite were prepared using a urea-assisted homogeneous precipitation method and characterized by XRD, FTIR, SEM, TEM, TGA, and DSC [1]. Preliminary results confirmed successful dopant incorporation, with non-doped HAp forming plates and rods, single-doped HAp appearing as needles, and multi-doped HAp forming compact spherical agglomerates (Figure 1), while the Ca/P ratio was critical to prevent carbonate or OCP impurities. These findings underscore the potential of multi-ion doped HAp as a bioactive material for bone tissue engineering.

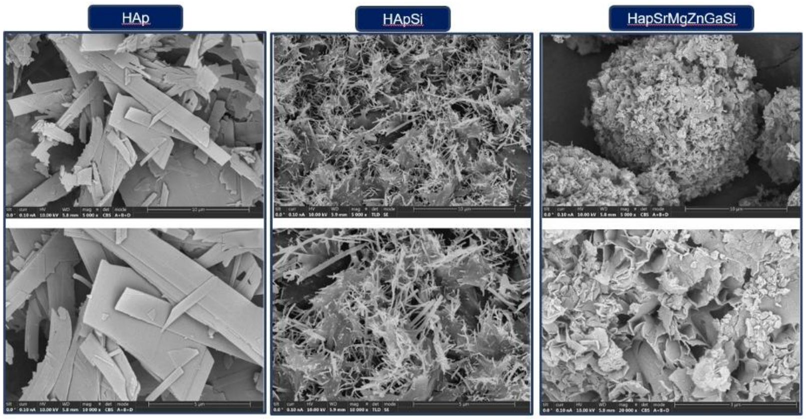

Figure 6. SEM images of non-doped HAp (left), Si-doped HAp (middle), and mHAp (Mg, Sr, Si, Zn, Ga) (right).

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Functionalized erythrocyte membrane vesicles as a novel drug delivery system for breast cancer treatment

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There has been considerable development in the field of biomimetic drug carriers in recent years. A particularly interesting type of carriers are erythrocyte membrane vesicles (EMVs), owning to their ductility, self-marking, tropism toward soft tissues and long circulation time. Further steps have been made toward active targeting by functionalizing EMVs with targeting agents. A promising target for breast cancer treatment is the Y1 receptor (Y1R) from the Neuropeptide Y (NPY) receptor family. In NPY receptor-positive breast cancers, Y1R is present in all tumour samples, compared to only 58% in normal breast tissue [1]. Therefore, functionalized EMVs with targeting agents for Y1R could serve as an active targeting strategy for breast cancer treatment. The aim of this study was to functionalize EMVs with an NPY analogue by utilizing several different lipid anchors and evaluate the differences in functionalization.

Human EMVs were generated via hypotonic lysis, followed by sonication and extrusion (Figure 1). An NPY analogue with enhanced binding affinity relative to native NPY was developed for surface conjugation, which was based on lipid insertion. PEG-maleimide-functionalized phospholipids of varying chain lengths and saturation (DSPE, DOPE, DPPE) were first conjugated to the NPY analogue via a maleimide–thiol reaction. This was followed by insertion of the lipid–peptide conjugates into EMVs. Finally, we characterized the samples with fluorescence intensity measurements, dynamic light scattering, transmission electron microscopy, and SDS-PAGE with silver staining.

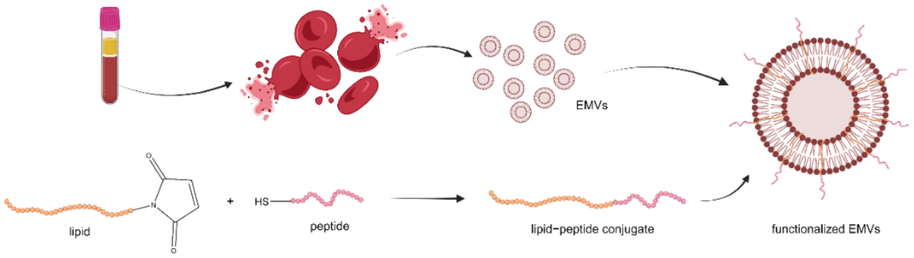

Figure 1. Lipid-peptide conjugation to EMVs. Created in BioRender.

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Self-ferroelectric and piezoelectric responses driven by giant interfacial strain gradient in BiFeO3/BaTiO3 superlattices

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Artificially engineered oxide superlattices provide a powerful platform to manipulate strain, interfacial coupling and ferroelectric/piezoelectric responses, enabling functionalities unattainable in single-phase films. We investigate 250-nm-thick $(BiFeO_3)0.65\Lambda/(BaTiO_3)0.35\Lambda$ (BFO/BTO) superlattices with modulation periods Λ = 24-195 Å grown by pulsed-laser deposition on $SrTiO_3$(001) buffered with a conductive $SrRuO_3$ bottom electrode. High-resolution X-ray diffraction atomic force microscopy and scanning transmission electron microscopy demonstrate phase-pure, smooth and highly epitaxial heterostructures with a well-defined nanoscale chemical modulation.

From the average lattice parameters, the BTO layers are compressively strained and exhibit enhanced tetragonality, whereas the BFO layers are tensile strained with a slight reduction of tetragonality relative to bulk. Beyond these average values, STEM-GPA strain mapping reveals pronounced interfacial strain gradients ($\sim 10^5$ m^{-1}) confined to the first ~30 nm above the SRO interface for $\Lambda \geq 95$ Å. These gradients correlate with a strong tetragonal distortion in BTO and local regions with $c/a > 1$ in BFO, together with the coexistence of rhombohedral-like and tetragonal-like BFO domains.

Ferroelectric and dielectric measurements show that short-period superlattices display enhanced polarization and dielectric permittivity. In contrast, long-period structures ($\Lambda \geq 95$ Å) develop a giant internal bias field ($E_s \approx -200$ kV/cm) that stabilizes a robust self-polarized state. Piezoresponse force microscopy confirms ferroelectric switching and reveals a self-piezoelectric response at zero external field, consistent with the strong built-in field induced by the interfacial strain gradient. The stabilization of this self-polarized piezoelectric state, combined with the reduced zero-field dielectric permittivity, provides a promising route to maximize figures of merit in lead-free oxide nanostructures for next-generation piezoelectric devices.

Magnetic-field-assisted printing of micro/nano devices for motor and sensing applications

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Additive manufacturing of polymer-bonded permanent magnets enables rapid prototyping and fabrication of complex geometries. However, conventional fused deposition modelling (FDM) typically yields isotropic magnetic properties because anisotropic Nd-Fe-B particles cannot be reliably aligned during extrusion [1], [2]. This limit printed components with tailored magnetization profiles for motors, sensors, and compact electromechanical devices.

This work introduces an FDM print-head concept that uses magnetic fields from all directions to precisely align magnetic particles as the material is printed, allowing better control over the final product's properties. A compact, water-cooled, multi-axis electromagnet array integrated around the nozzle generates localized magnetic fields with programmable magnitude and three-dimensional orientation. Micro-Hall sensors near the printing area measure magnetic fields in real time and automatically adjust the applied field to keep it accurate, improving alignment accuracy and repeatability [3]. The magnetic field is timed with the printer's movement and the material's cooling so it can act before the material hardens.

Figure 1. Proposed design of print head.

The proposed system is expected to enable spatial control of particle easy-axis orientation and fabrication of radial, multipolar, and Halbach-like magnetization patterns without external fixtures or post-process alignment [3]. Designed for polymer-bonded anisotropic Nd-Fe-B feedstocks, including recycled powders, the concept supports circular-material strategies and offers a scalable route to higher-performance printed magnets for motor and sensing applications [4].

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Influence of hot deformation on corrosion behaviour and zirconium conversion coating formation of AlSi10Mg alloy

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In a world built on different metals and alloys, there is a constant risk of material failure. One of the most common threats is the spontaneous process of metal degradation known as corrosion. To prevent material failure, various protection methods have been developed, including conversion coatings. Due to the toxic nature of highly efficient chromate conversion coatings, more environmentally friendly zirconium-based conversion coatings (ZrCC) have been developed. Since conversion coatings typically initiate and grow around intermetallic particles (IMP) and surface defects, the surface quality, pretreatment of the substrate material, and its chemical composition play important roles in the quality and protective efficiency of these coatings.

For this study, wrought aluminium alloy 4004 (AlSi10Mg) was produced using two different processing routes. The first set of samples was prepared by casting, while the second set was also cast and subsequently hot-deformed at 450 °C. Two sets of samples with different microstructural characteristics were obtained (Figure 1a and 1b). ZrCC formation begins at IMPs and defects, which can lead to an uneven and locally cracked coating on the cast surface (Figure 1c). In contrast, the deformed samples exhibited finer microstructural features and lower porosity, resulting in a more uniform coating (Figure 1d).

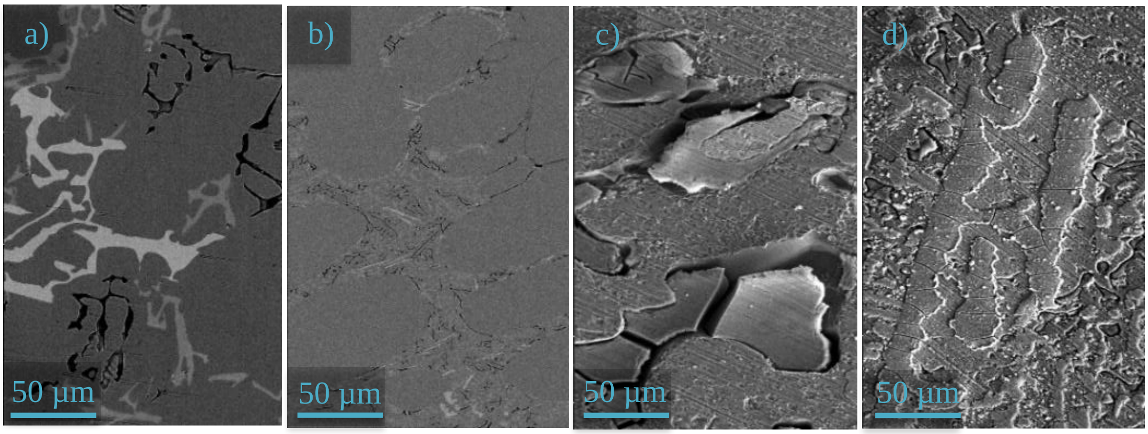

Figure 1. Microstructure by scanning electron microscopy a) cast microstructure b) cast microstructure after hot deformation c) ZrCC on cast microstructure and d) ZrCC on deformed microstructure.

Magnetically Actuated Biocidal Nanorods for Biofilm Eradication

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Magnetic nanomaterials have attracted considerable interest for biomedical applications due to their tunable physicochemical properties and responsiveness to external magnetic fields. In particular, superparamagnetic iron oxide nanoparticles (SPIONs) enable remote actuation and targeted interactions with biological systems [1]. These features make them promising candidates for addressing microbial biofilms, which exhibit high tolerance to antimicrobial treatments and contribute to persistent infections [2]. By combining magnetic actuation with surface functionalization, such nanoparticles can mechanically disrupt biofilm structures while enhancing antibacterial activity [1].

In this work, anisotropic magnetic nanorods were prepared for magnetically driven disruption of microbial biofilms combined with antimicrobial surface activity. SPIONs were used as building blocks and assembled into elongated nanorods under an external magnetic field, followed by silica coating to stabilize the anisotropic structures. The resulting nanorods exhibited an average length of approximately 1.9 ± 0.7 μm and retained superparamagnetic behavior. To introduce antimicrobial functionality, the silica surface was modified with cationic ligands using silane coupling and click chemistry reactions. Surface modification was confirmed by zeta potential analysis, which showed shifts in the isoelectric point from 3.5 for bare nanorods to 8.4–10.7 after ligand attachment. Nanoparticle morphology, colloidal stability, and surface properties were characterized using transmission electron microscopy, vibrating sample magnetometry, dynamic light scattering, and zeta potential measurements.

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Fascinating structural diversity and catalytic properties of CuCl-based coordination polymers

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Cupro(I) chloride coordination polymers are a widely studied class of compounds, exhibiting versatile structural geometries [1] and a wide range of physicochemical properties [2]. The use of rigid N-ditopic co-ligands, such as DABCO (triethylenediamine), as linkers and charge-ion transporters, expands the structural diversity and properties of CuCl-based networks [3]. However, current publications cover relatively few such coordination compounds and provide limited information, such as crystal data and molecular structure [4].

Solvothermal syntheses were carried out at 130-150 °C for 5 days. $CuCl_2$ and copper powder (for *in situ* formation of Cu(I)), HCl, and DABCO were used as starting reagents, with ethanol or methanol as solvents. After cooling to room temperature, orange plate crystals of Cu_3Cl_6(DABCO) (space group $P2_12_12_1$, Z=2) and colourless rhombohedral crystals of [N, N´-$Me_2DABCO^{2+}]_2[Cu_9Cl_{13}]^{4-}$ (Me = methyl) (space group *I2/a*, Z=8) were obtained at the bottom of a Teflon liner. The inorganic parts in these compounds are represented as 2- and 3-dimensional cupro(I)chloride networks respectively, It should be noted that during the synthesis of Compound 2, the solvent molecules react with DABCO, forming N,N´-Me_2DABCO^{2+} quaternary dications *in situ*. The synthetic conditions and stoichiometry were optimized to achieve the highest possible crystalline product yields.

The obtained compounds were characterized by single-crystal X-ray diffraction and Raman spectroscopy. The catalytic properties of both compounds were also studied in the mild oxidation of alkanes, as well as in C–C and C–N coupling reactions. The catalytic reaction products were identified using GC-MS. Product yields and reaction kinetics were examined by GC-FID and UV-Vis spectroscopy. In conclusion, further investigation is required to fully understand the other physicochemical properties of the obtained compounds.

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Local lattice parameters through sub-pixel refinement of STEM images

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Advances in high-resolution STEM imaging now make it possible to routinely obtain atomic-level images at 10 pm/px. Such imaging enables the investigation of stress, strain, polarization, and material defects at the level of individual atoms. However, converting these images into quantifiable data requires specialized software and analytical methods.

In this work, we present a new approach for quantifying local lattice parameters through sub-pixel refinement. Through a series of processing steps (Figure 1), raw images are transformed into analyzable data sets. These data then enable analyses including local ellipticity, edge-length comparison, local displacement, and c/a mapping.

To support this workflow, we developed STEMliner, a new software solution based on the scikit-image and SciPy libraries. With particular emphasis on rapid, automated refinement and peak classification. as well as script based automatic visualization of the results, STEMliner is comparable to other state-of-the-art software packages.

The method has already proven useful for determining strain and dislocations in diverse systems, including Ge single crystals, $SrTiO_3$ perovskite thin films, and natural garnet minerals. Further development is planned to improve accessibility, reproducibility, and availability to the wider community.

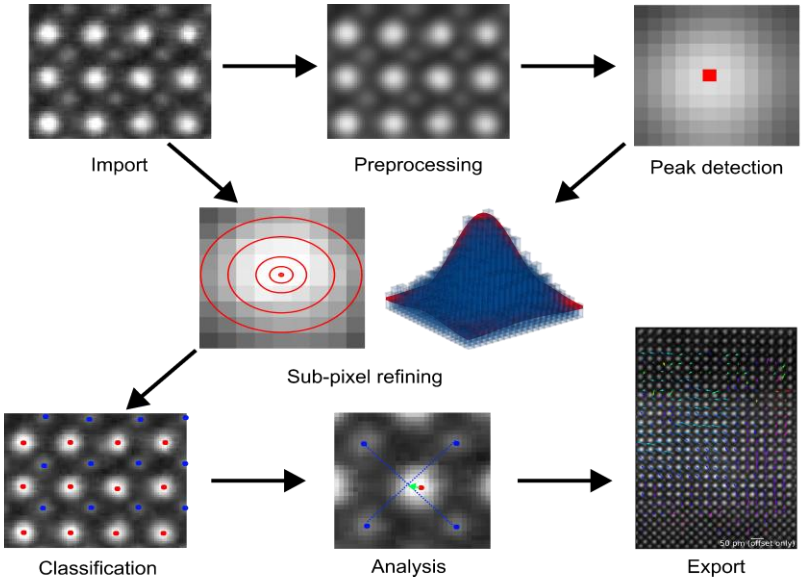

Figure 1. The process of determining local lattice parameters at the atomic scale

Effects on SFO Sintering

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The stability and sintering behavior of $SrFe_{12}O_{19}$ (SFO) are strongly dependent on the surrounding atmosphere and the presence of reductive materials, which can act as reducing agents and trigger metastable phase formation [1,2]. TGA and DSC are effective techniques for monitoring mass changes and phase transitions during heating, providing insights into decomposition, sintering, and chemical reduction processes. The interplay of temperature, atmosphere, and carbon content is therefore crucial for predicting densification, microstructure evolution, and magnetic performance. Pure SFO and SFO with 10 wt% graphite (SFO+C) were heated and examined under air, argon, and vacuum by TGA/DSC. Pure SFO in vacuum and inert gas remained stable up to ~700 °C, with only minor mass loss due to surface-bound water evaporation, and exhibited broad endothermic events around 800–1000 °C corresponding to densification and minor phase relaxation. In SFO+C, mass loss of up to 12 % was observed between 650–1200 °C in inert and vacuum atmospheres, associated with pronounced endothermic peaks indicating carbothermal reduction and formation of Fe_3O_4, α-Fe, γ-Fe, and oxygen-deficient Sr–Fe oxides [1]. In air, a slight mass increase below 600 °C was observed, indicating initial reoxidation, followed by exothermic peaks corresponding to hexaferrite stabilization. Microstructural analysis pSPS sintered sample at 1300 °C / 5min revealed that Sr-rich secondary phases formed liquid layers surrounding grains, facilitating partial liquid-phase sintering and localized densification, while some regions exhibited porosity and microcracks due to uneven mass transport. The thermal events in DSC, together with heterogenous microstructural changes, indicate that reduction, densification, and partial melting occur simultaneously in carbon-containing samples, emphasizing the strong influence of carbon content on sintering pathways, phase stability, and magnetic properties. Atmosphere however also plays an important role in phase stability at sintering temperatures.

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Tri-metallic boride catalysts for efficient sea water electrolysis

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The transition from fossil fuels to clean renewable energies is essential to mitigate the global carbon emissions. Hydrogen produced by water electrolysis using renewable energies is a great alternative for fossil fuels. The emerging Anion Exchange Membrane (AEM) water electrolyser combines the pros of conventional alkaline water electrolyser (AWE) and commercial proton exchange membrane (PEM) water electrolyser in terms of low cost and efficiency. The commercial water electrolysis mainly uses pure water feed which can affect the global pure water availability and the operating cost. Replacing the pure water feed with low grade water sources such as widely available sea water is a promising solution[1]. Competitive chlorine evolution reaction (ClER) over oxygen evolution reaction (OER), low performance, and degradation of the catalysts are the main challenges of sea water electrolysis.

Herein, we used a combination of low cost Co, Fe and Mo boride catalysts to tackle the challenges of sea water electrolysis [2], [3]. The optimisation of the crystallinity and activation of the catalyst improved the catalytic activity. The crystalline CoFeMoB catalyst showed good corrosion resistance and OER selectivity with an overpotential of 436mV at 10mA/cm^2 in synthetic sea water (pH 12). This preactivated catalyst sustained 50 hours of chronoamperometric stability test at 1.7V (vs RHE) without any corrosion. The trimetallic boride catalyst offers good promise for further investigations and implementation in sea water electrolysis.

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Synthesis, characterization, and electrochemical evaluation of CuO-Decorated Carbon for Mg-S Batteries

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Magnesium sulfur (Mg-S) batteries are promising next-generation energy storage systems due to their high energy density, abundant materials, and lower environmental impact. However, their use is limited by slow sulfur redox kinetics, poor reversibility, and the polysulfide shuttle effect [1]. This study investigates the effect of CuO decoration on carbon-sulfur cathodes to enhance the electrochemical performance of Mg-S batteries. Commercial ENSACO carbon was decorated with varying amounts of CuO (1, 5, and 10 wt%) and infiltrated with sulfur (S_8) to form composite cathodes. The materials were characterized using XRD, XPS, and electron microscopy. Swagelok-type Mg-S cells were assembled using magnesium metal as the anode and the prepared composites as the cathode, with $Mg(TFSI)_2/MgCl_2$ in diglyme as the electrolyte. Galvanostatic cycling with potential limitation was performed to evaluate battery performance. Additionally, *ex situ* XES was used to monitor the average charge on sulfur and determine relative amounts of different sulfur species produced electrochemically within the cathode at different stages of cycling [2]. CuO-containing cathodes show improved cycling stability and higher discharge capacity than pure sulfur systems, consistent with known sulfur reduction mechanisms [3]. Combined electrochemical and spectroscopic analysis provides deeper insight into the sulfur conversion, contributing to the development of more efficient and sustainable metal-sulfur battery technologies.

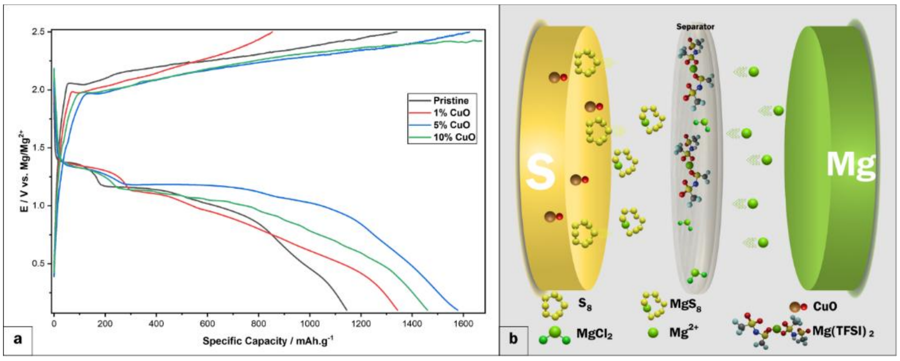

Figure 1. (a) First discharge/charge voltage profiles of Mg–S cells at C/10. (b) Schematic of the Mg–S battery configuration and reaction mechanism.

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Ascorbic acid-assisted green hydrothermal synthesis of ZnO thin films for enhanced photocatalytic performance

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Zinc oxide (ZnO) thin films are promising photocatalytic materials for environmental remediation; however, achieving controlled morphology and reproducible performance remains a key challenge. The use of environmentally friendly additives offers a sustainable approach to tailoring growth mechanisms and material properties.

In this work, ascorbic acid is introduced as a green modifier during the hydrothermal synthesis of ZnO thin films at 90 °C from a zinc nitrate aqueous solution. A concentration-dependent study shows that ascorbic acid strongly influences the growth regime, defining a narrow operational window (~3 mM) in which continuous film formation is preserved.

The photocatalytic performance of the synthesized films was evaluated through the degradation of a model pollutant under simulated solar irradiation using UV–Vis spectroscopy. Enhanced photocatalytic activity was observed after post-synthesis annealing (600 °C, 2 h); annealed samples exhibit higher degradation rates compared to non-annealed films.

Complementary structural and morphological characterization was carried out using scanning electron microscopy (SEM) and X-ray diffraction (XRD) on both annealed and non-annealed samples. These analyses aim to establish correlations between synthesis conditions, film structure, and photocatalytic performance.

This work demonstrates the potential of green modifier-assisted synthesis for tuning ZnO thin films and provides a basis for the development of more reliable photocatalytic systems for environmental applications, including the degradation of emerging pollutants and microplastics.

Additive manufacturing of thick ceramic parts

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Additive manufacturing of ceramics has gained attention as one of the few methods capable of producing highly complex geometries. Among these, Vat Photopolymerization (VPP) techniques enable details unattainable by other methods. Nevertheless, “complexity for free”, often promised with additive manufacturing, is only partially fulfilled. In ceramic VPP, design freedom remains limited, making design for additive manufacturing not only an opportunity, but a necessity.

These limitations are largely a consequence of the debinding step, during which the organic components necessary for the 3D printing process are removed. It remains one of the most critical challenges, involving exothermic polymer oxidation and rapid gas evolution, leading to heat and pressure build-up within the part. As a result, thin-walled structures are typically required to prevent cracking.

In this presentation, we introduce a simple slurry formulation approach that significantly alters debinding behaviour. It enables faster processing and allows for centimeter-thick walls, while maintaining a conventional debinding process in air.

High-Pressure Ammonia Synthesis using Co–Ni@CeO_2 Magnetic Nanocomposite Catalysts: Synthesis, Activity and Stability

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Approximately 85 % of the globally synthesized ammonia (by Haber–Bosch process) is used for the manufacture of synthetic fertilizers [1], making it essential for modern agriculture. The Haber–Bosch process traditionally use iron-based catalysts and, more recently, expensive ruthenium-based catalysts, which operate under high temperature (300–500 °C) and pressure (50–200 bar) conditions. Magnetic heating has recently emerged as a promising alternative approach for catalytic processes, enabling localized heating of magnetic nanoparticles (NPs). This method can potentially enhance reaction efficiency consequently reducing overall energy consumption compared to conventional heating methods.

In this work, $Co_{0.67}Ni_{0.33}$ alloy NP decorated with cerium(IV) oxide nanoparticles (Co-Ni@CeO_2) were investigated as potential magnetic catalysts for ammonia synthesis. The catalysts were prepared using a Pechini sol–gel method [2], followed by reductive heat treatment. The influence of citric acid concentration and reduction temperature on the magnetic and catalytic properties of the prepared nanocomposites was systematically investigated. The best performing nanocomposite, reduced at 600 °C in a hydrogen atmosphere, exhibited a magnetic saturation of 65 emu g^{-1} (measured by Vibrating-sample magnetometer) and a specific absorption rate (SAR) of 17.8 W g^{-1} under an alternating magnetic field (30 mT, 300 kHz, measured by AC magnetometer).

The Co-Ni@CeO_2 catalyst was tested across different reaction temperatures under ammonia synthesis conditions in an alternating magnetic field (234 kHz, Fig 1.). Catalyst achieved a maximum ammonia synthesis rate of 19.4 mmol NH_3 g_{cat}^{-1} h^{-1} at 600 °C and 55 bar, while maintaining stable operation for 24 h.

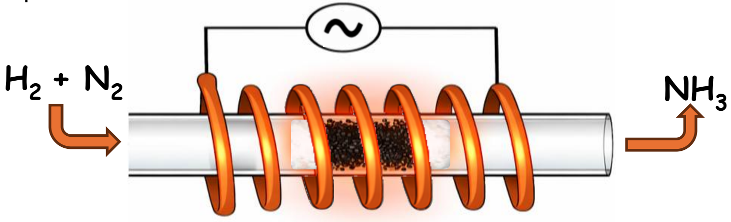

Fig 1. Schematic illustration of magnetically heated reactor.

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Atomistic insights into chloride-induced copper removal at surface defects

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Dissolution of copper induced by chlorides is a key factor in its localized corrosion and passive film breakdown [1]. It is known that, even under ultra-high vacuum (UHV) conditions, Cl desorbs as CuCl [2], whereas in the aqueous phase copper dissolution proceeds via the release of $CuCl_2^-$ complexes [3]. To elucidate the underlying mechanisms in both environments, we investigated the desorption of Cl from a kinked copper surface, Cu(11 7 5), using density-functional-theory calculations. Our calculations reproduce the experimentally observed formation of CuCl during desorption in vacuum and $CuCl_2^-$ during dissolution in aqueous solution (Figure 1), providing a unified atomistic picture of chloride-induced copper removal. These insights provide a foundation for future, more application-oriented studies addressing the role of corrosion inhibitors — substances that reduce the corrosion rate of metals — in mitigating chloride-induced copper dissolution.

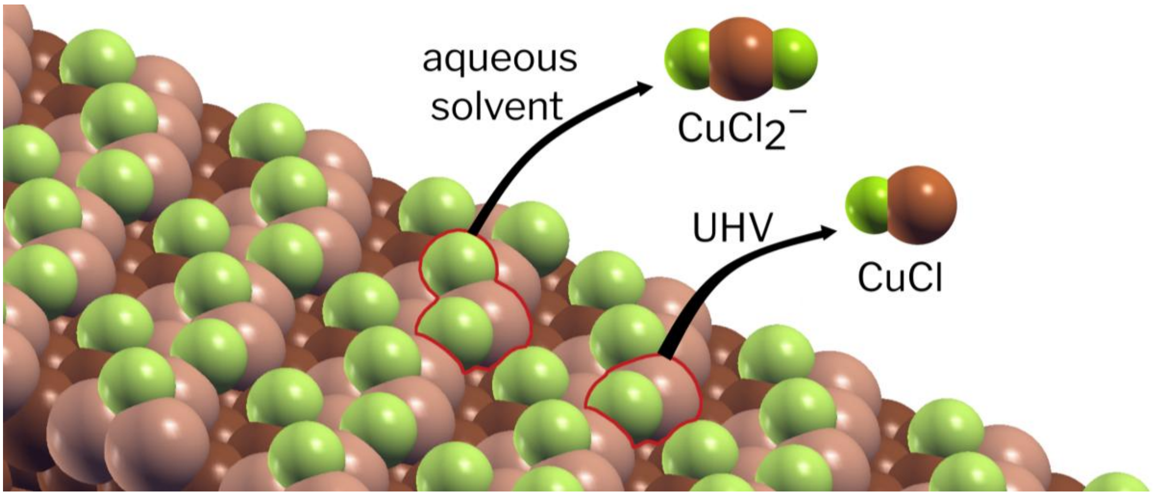

Figure 1. Illustration of chloride-induced Cu removal from the Cl-covered kinked Cu(11 7 5) surface, showing CuCl desorption in vacuum and $CuCl_2^-$ detachment in aqueous solution. Cl atoms are shown in green, while lightly colored Cu atoms indicate step-edge sites.

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Influence of defects in $Bi_4Ti_3O_{12}$ platelets on their transformation into $SrTiO_3$ with preserved 2D morphology

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Comprehension of the atomic-scale microstructure of $Bi_4Ti_3O_{12}$ (BIT) platelets is crucial for understanding and controlling their hydrothermal transformation into $SrTiO_3$ (ST) platelets with tuned surface and functional properties. Two types of $B_4Ti_3O_{12}$ (BIT) nanoplatelets were prepared by the molten salt method: one nearly defect-free and the other containing several microstructural defects. These BIT platelets then served as the template for the conversion into $SrTiO_3$ (ST) under an alkaline hydrothermal method at 200°C, with varying NaOH concentrations, Sr excess, and reaction times. In the BIT-to-ST transformation, non-defective BIT requires a low strontium (Sr/Ti = 3) excess to preserve the 2D morphology. This can be explained by the high structural matching between BIT and ST, together with their appropriate relative solubilities, which allows the transformation to proceed via BIT dissolution from the lateral side and epitaxial growth of ST over the basal planes of the BIT template, resulting in ST platelets that retain the 2D morphology of BIT. Under the same conditions, defective BIT platelets undergo complete disintegration, yielding irregularly shaped ST particles. But, at a higher Sr (Sr/Ti = 24) excess, a defective BIT template can also be transformed into ST with a preserved 2D shape. The differences in the transformation mechanisms and morphological development will be discussed in the context of nucleation–crystallization theory and atomic-scale STEM observations [1]. As prepared materials will be evaluated for catalytic alcohol conversion and photocatalytic H_2 production to understand their functional properties in correlation with the surface characteristics.

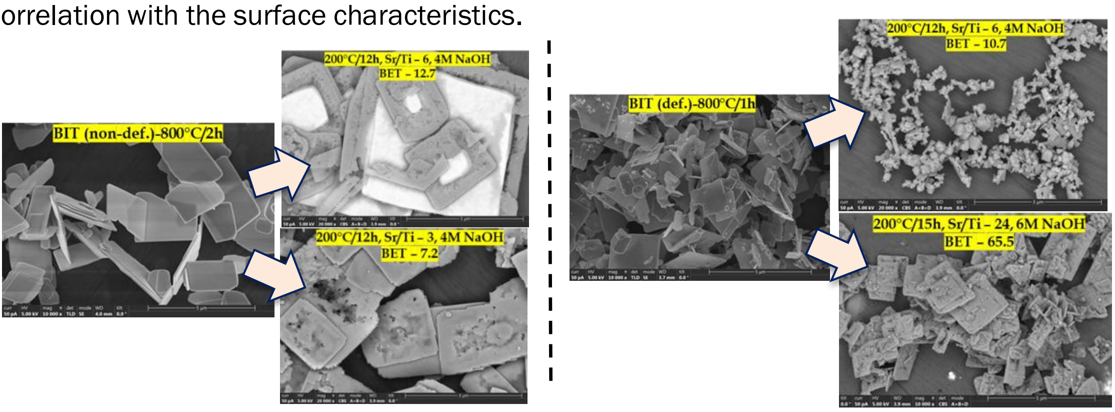

Figure 1. BIT (defective and non-defective) to ST transformation

References

No spore left uncounted: challenging fungi and dPCR assays

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Life finds a way – even in the harshest of environments, like solar panels. While fascinating, the formation of biofilms on solar panels causes significant losses in power production. To effectively reduce their impact, we first need to understand what, and how much of it, grows in these biofilms. Molecular biology has come a long way in helping uncovering species diversity and quantification of microorganisms in variety of samples. But measuring biological substances is a relatively new and much more complicated concept compared to physical and chemical measurements. Although several methods for measuring microorganisms exist, PCR technology, more precisely digital PCR (dPCR), has become increasingly important for this purpose.

Fungi are the dominant organisms in solar panel biofilm communities, and most of them are underrepresented in research. We selected four presumably core solar panel-inhabiting fungi as our model organisms for DNA based investigation of their presence. To be able to measure them with dPCR we first needed to identify what we will measure – a species-specific, single-copy sequence of their DNA. Our workflow was quite quickly disrupted by the lack of available DNA sequence data that was crucial to designing purpose-specific assays. Nevertheless, with quite some modifications to the pipeline, we were able to design and evaluate dPCR assays for three out of the four fungi. The assays were characterized and validated on synthesized DNA fragments and DNA extracts of fungal isolates. Finally, the validated assays will be used on real-life samples that will be collected with the help of citizens (Figure 1) in a citizen science project to gain insight into solar panel fungal communities of Slovenia.

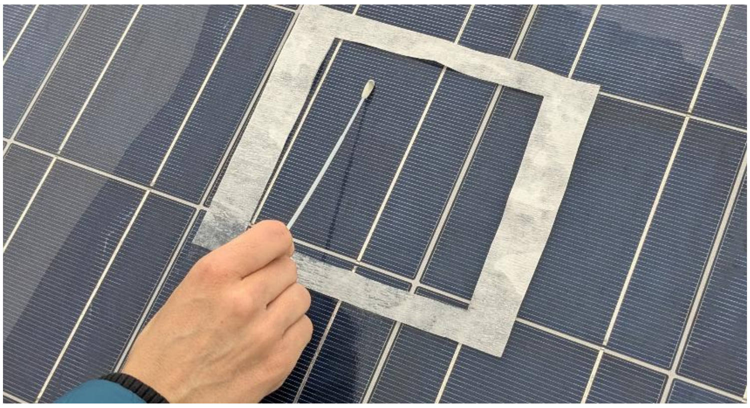

Figure 1. Sampling of solar panel biofilms.

Effect of surface oxidation of SiC powders on the properties of photocurable suspensions

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Digital Light Processing (DLP) vat photopolymerization is an additive manufacturing technique used to produce ceramic components with high dimensional accuracy and good surface finish. The technology is well established for several oxide ceramics, such as SiO_2, Al_2O_3, and ZrO_2. However, the processing of non-oxide ceramics remains challenging. In particular, silicon carbide (SiC) exhibits strong light absorption and a high refractive index mismatch between the ceramic particles and photopolymerizable monomers, which significantly limits curing depth, accuracy and overall printability.

To address these challenges, this work aims to investigate the surface modification of SiC powders via controlled thermal oxidation as a strategy to improve their suitability for DLP processing. Several commercial SiC powders were selected to study the influence of particle size, size distribution, and polytype on the oxidation behavior and subsequent photopolymer suspension properties. Surface oxidation was carried out at different temperatures, following by characterization of oxidized powders in terms of mass change analysis, particle size and specific surface area evaluation. Thickness of the formed oxide layer was determined using electron microscopy. Light absorption in the UV–Vis range was analyzed to assess changes in optical properties of modified powders.

Based on the modified powders, ceramic suspensions with up to 50 vol.% of solids loading were formulated and evaluated in terms of sedimentation stability, viscosity and curing depth. Finally, printing trials were performed using a DLP printer (CeraFab S65, Lithoz, Austria) to correlate powder properties and oxidation conditions with printability. This study is expected to provide a fundamental understanding of surface oxidation in improving curing depth and accuracy in SiC-based DLP suspensions, contributing to the advancement of non-oxide ceramic additive manufacturing.

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Inverted pyramid evolution on the Ge (001) surface via thermal etching

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Surface modifications in semiconductors that result in pyramidal morphologies are widely used in photovoltaics and (photo)electrocatalysis, where they enhance light absorption through increased scattering and improve catalytic performance [1]. Conventional fabrication methods rely on wet chemical etching, which raises environmental concerns [2]. In this work, inverted pyramids were formed on a Ge (001) surface without the use of chemical etchants. Thermal etching was performed at 550 °C in a low-pressure oxygen atmosphere (10^{-5} mbar) within a vacuum chamber. Oxygen exposure leads to the formation of GeO$_X$, which becomes thermally unstable above 500 °C and desorbs during annealing, resulting in material removal and pit formation that evolves into inverted pyramids[3]. Atomic force microscopy reveals that pyramid size and depth increase with etching time, reaching depths of up to 400 nm. With further growth, the pyramids begin to coalesce, forming interconnected trench-like structures (Fig. 1). Optical measurements show reduced reflectance at a wavelength of 488 nm, indicating enhanced light absorption in the visible spectrum due to the modified surface geometry. These results demonstrate an environmentally friendly and controllable approach to surface structuring for improved light management in Ge-based solar or photoelectrochemical cells.

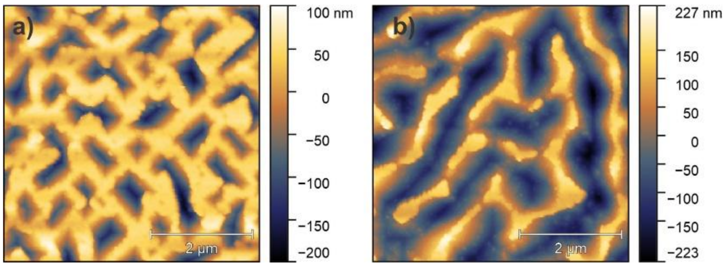

Figure 1. Germanium surface with separated inverted pyramids (a) and with interconnected inverted pyramids (b).

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Evaluation of molecular gas transport models in microcapillaries

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Molecular gas transport through microcapillaries becomes increasingly complex in rarefied conditions and very small diameter tubes, where the flow transitions from continuum to free molecular regimes and classical descriptions lose validity. The intermediate slip and transitional regimes are particularly challenging due to strong dependence on pressure, geometry, and gas properties, as well as spatial variations of the Knudsen number along the channel [1,2]. No single low-complexity or analytical model accurately captures mass flow across the full range of pressures and diameters, as local transitions in flow regime occur along the capillary. Existing models assume a uniform regime, while real capillaries at very low diameters exhibit spatially varying regimes [2-4].

Our work investigates gas flow through microcapillaries with diameters ranging from 2 to 200 μm, connecting a controlled inlet pressure to a vacuum-pumped outlet. Five different gases are examined to assess the influence of molecular properties on transport behaviour. The study focuses on testing and evaluating existing flow descriptions, which range from continuum with slip corrections to rarefied models, in order to identify relations that best capture the experimentally observed mass flow under varying conditions. The primary objective is to establish a reliable framework for predicting mass flow as a function of gas species, capillary diameter, and inlet pressure, accounting for regime transitions along the channel. Such a model is relevant for applications requiring precise and controlled gas delivery into vacuum environments, where direct measurement of throughput is often not feasible.

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Room temperature nucleation of confinement-induced borophene seeds for next-generation energy storage

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Borophene has good potential as a high capacity electrode material for next generation energy storage devices. However, its widespread application is hindered by rapid environmental degradation and reliance on high temperature, metal catalyzed synthesis under ultrahigh vacuum conditions. Through an Italy-Slovenia collaboration via the Erasmus Mundus Master GREENANO, we report metal free, room temperature nucleation of borophene seeds confined within a van der Waals (vdW) gap. Following established room temperature intercalation protocols [1], thermal evaporation of boron onto air cleaved HOPG revealed the formation of unexplained subsurface nanoscale blisters under scanning tunneling microscopy (STM). To explain this phenomenon, comprehensive vdW corrected density functional theory calculations modeled boron clusters (B1 to B18) intercalated within a macroscopic graphite supercell. Our thermodynamic analysis reveals that the energetic competition between host-intercalant binding and the graphite lattice's elastic deformation penalty drives a novel structural phase evolution. While small boron clusters are naturally planar in a vacuum, graphitic confinement forces them to crumple into 3D geometries. The calculated geometry for the intercalated B8 cluster produces a localized blister height of 0.1629 nm and a width of 2.58 nm, matching the experimental STM measurements of 0.163 nm and 2.6 nm with significant accuracy. As the cluster grows to B18, internal covalent cohesive forces overcome the out of plane vdW forces, emerging as a flat borophene embryo. This confinement induced 2D nucleation offers a new pathway to synthesize zero metal borophene-graphene heterostructures, addressing bottlenecks in scalable energy storage.

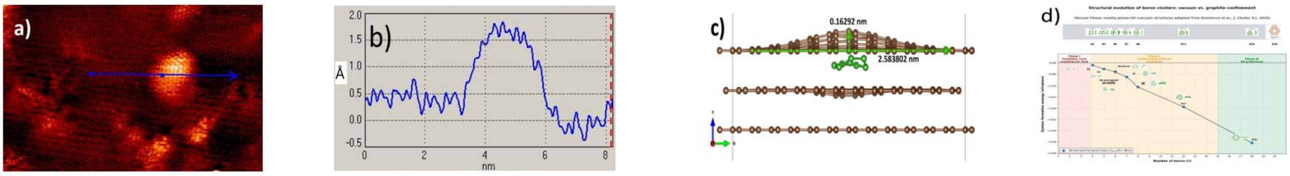

Figure 1. Experimental STM and line profile of blister (a, b), theoretical match with B8 (c), structural evolution and formation energy curve of boron nanoclusters in vacuum versus graphitic confinement (d)

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Full capsids matter: towards optimized rAAV production with focus on vector genome integrity

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Recombinant adeno-associated viruses (rAAVs) are leading vectors used in gene therapy, yet their therapeutic efficiency is frequently limited by viral particles containing fragmented or incomplete genomes. A better understanding of the factors that influence viral genome integrity is therefore critical for improving vector quality and safety. In this study, we made a first step towards optimization of transfection parameters to enhance viral vector yield and increase complete viral genome titers. Recombinant AAV9 samples were produced using triple transfection of HEK293T suspension cells (Figure 1). After harvesting, capsid titers of crude lysates were quantified using ELISA, and a multiplex digital PCR targeting four genomic regions was used to determine the number of complete genome titers. In initial small-scale production experiments, we compared the performance of two different transfection reagents, FectoVir (Sartorius) and KyFect (KyFora Bio). Using default transfection protocols recommended by the manufacturers of each reagent, KyFect provided higher complete genome titers compared to FectoVir. Adjusting the plasmid ratio of FectoVir substantially improved the number of complete genomes. We further evaluated the scalability of the system using two different culturing systems – shaker flask and a bioreactor. Cells cultured in shaker flask exhibited higher viability than cells grown in bioreactor, consequently both the capsid titer and complete viral genome titer were significantly higher in samples produced in shaker flask. These results demonstrate that there is room for additional optimization to obtain a robust rAAV9 production platform that will in future enable systematic investigation of key factors involved in viral genome integrity. Although shaker flasks outperformed the bioreactor in initial scale-up experiments, bioreactors remain the preferred platform for large-scale rAAV manufacturing, highlighting the need for further optimization of bioreactor culturing conditions and rAAV production.

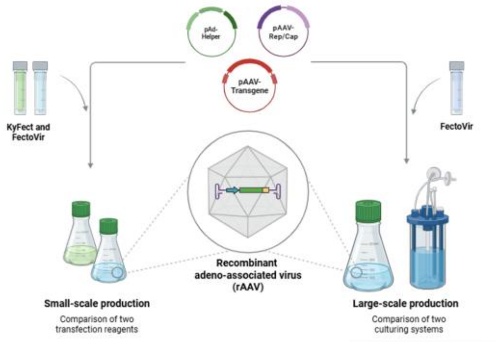

Figure 1. Optimization of rAAV production process (Created in BioRender.com).

Hydroxylation-driven boron dissolution in Co-borides: a DFT study

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ulti-metallic boride nanoparticles are promising precatalysts for the oxygen evolution reaction (OER), yet significant boron leaching is consistently observed during their initial structural transformation under OER conditions [1]. To elucidate its atomistic origin, we performed density-functional theory (DFT) calculations. We first showed that incorporation of B into Co-based metallic phases is energetically unfavorable, providing a thermodynamic driving force for boron segregation toward the surface. At the surface, when O and B are co-adsorbed, the B–O interaction is significantly stronger than both Co–O and Co–B bonding, driving the formation of a two-dimensional B_2O_3-like overlayer that weakly binds to the surface and can detach. More importantly, under hydroxylated conditions, OH groups preferentially coordinate to surface boron, leading to the spontaneous formation of $B(OH)_3$ units. These units readily desorb (Figure 1), revealing an intrinsic thermodynamic driving force for hydroxylation-induced boron dissolution. This behavior explains the experimentally observed boron leaching and identifies $B(OH)_3$ formation as the key intermediate governing boron removal. The results provide an atomistic rationale for the sacrificial role of boron, where surface boron species are selectively oxidized and removed, thereby exposing active transition-metal sites that transform into the OER-active oxyhydroxide phase.

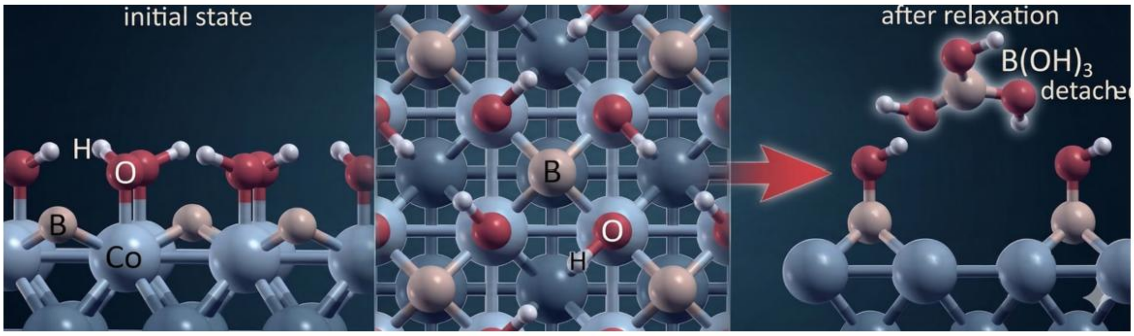

Figure 1. Structural relaxation of a B-covered Co(100) surface in the presence of OH groups (left and middle), showing formation and detachment of a $B(OH)_3$ species (right).

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Formation and Characterization of TiO_2 Nanotubes on DED-LB and Wrought Ti-6Al-4V Alloys with Copper Addition

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Orthopedic implants are medical devices designed to replace or support damaged bone structures, thereby improving patients' quality of life [1]. The Ti-6Al-4V alloy is widely used due to its favorable mechanical properties, low density, excellent biocompatibility, corrosion resistance, and ability to promote osseointegration [2,3]. This study investigates the formation of self-organized TiO_2 nanotubes on bare Ti-6Al-4V, as well as on alloy containing 4 wt.% Cu, produced by laser beam directed energy deposition (DED-LB), and compares them with conventionally wrought alloy. Anodization was performed in an ethylene glycol-based electrolyte containing NH_4F and H_2O using a two-step process at 20 V for 2 h. Microstructural and surface characterization were carried out using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX). Electrochemical behavior was evaluated using electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP). In vitro osseointegration was assessed by immersing thermally treated samples in Kokubo's simulated body fluid (SBF) at 36.5 °C for 28 days, followed by analysis of hydroxyapatite formation using SEM. The DED-LB alloys exhibited irregular and partially deformed nanotube structures due to α' martensitic microstructure and surface heterogeneity, whereas the wrought alloy showed uniform nanotubes. Electrochemical results confirmed enhanced passivation behavior for all samples, with the DED-LB alloys demonstrating superior stability. The results highlight the influence of additive manufacturing-induced microstructures on nanotube morphology and osseointegration, while Cu addition is expected to improve antibacterial properties [4].

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De novo design of anchors that bind to the termini of designed protein fibers

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Protein nanomachines carry out a wide range of functions in living organisms, driving essential cellular processes such as cell division, structural maintenance, and intracellular transport. With recent developments in protein design, it may be possible in the near future to create a system comprised entirely of proteins that would mimic natural protein nanorobots – for example, protein motors. We approach this by designing a system comprised of two main components: self-assembling fiber tracks and symmetrical oligomeric walkers that bind to the tracks via the orthogonal coiled-coil interactions and move along them.

In this work, we aim to design symmetric oligomeric anchors that would specifically attach to fiber ends, enabling controllable and directed fiber growth and attachment.

We first set out to design symmetric oligomers using RFDiffusion for backbone design, ProteinMPNN for sequence design, and AlphaFold2 for the structural validation of the model. After multiple rounds of computational design, we selected the best-ranking oligomers for experimental evaluation. We tested their oligomeric state using HPLC, mass photometry, and Cryo-EM, and for most designs observed a formation of higher-order assemblies, with molecular weight 2 or 3 times larger than intended; this effect was partially mitigated by fusing the soluble spydersilk domain to the protomers.

The top-performing candidates were then used as a part of designed anchors, where each monomer of a symmetric oligomer was fused to a fiber “cap” via flexible linkers of varied length. The caps were generated by redesigning one of the interaction interfaces within fiber monomers, enabling them to bind fiber ends and prevent further assembly at the same time. The interactions between these anchors and de novo–designed fibers were evaluated in vitro using TIRF microscopy to assess anchor assembly, behavior, and their colocalization with fiber termini.

Sensor Technologies

Survival and transmission risk of stable plant viruses in insect frass used as fertilizer

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With an increasing human population, the need for improved food production systems is growing, and fertilizers are an essential part of this process. Production of fertilizers by insect-mediated bioconversion has recently emerged as a novel solution for reusing organic waste, with fewer adverse environmental effects in comparison with conventional methods. Insect frass is a by-product of this process which consists of insect excrements, moulted skins, leftover food, and dead insects. Many studies confirmed its fertilizing properties, but the potential risk of transmitting plant pathogenic viruses to healthy plants via frass derived from insects fed on virus-infected plant material has not yet been investigated. In this study, we aim to determine the survival of stable plant viruses in insect frass and their potential to infect healthy plants. Insect frass was produced by rearing black soldier fly larvae on chicken feed mixed with tomato leaves contaminated with tobacco mosaic virus (TMV) and tomato bushy stunt virus (TBSV) (Figure 1). After gently drying the frass at low temperature and heating half of it for 1 hour at 70 °C following Regulation (EU) 2021/1925, we tested the samples for TMV and TBSV using reverse transcription real-time PCR (RT-qPCR). Heat-treated and non-treated frass were mixed with growing substrate (1:9 ratio) and used for sowing seeds and planting tomato seedlings, and the remaining frass was used for mechanical inoculation of healthy tomato plants. Monthly photographing and RT-qPCR testing of the plants over four consecutive months is currently in progress. The data that will be generated in this experiment will provide insight into the potential role of insect frass in the transmission of stable plant viruses and contribute to the assessment of its safe use as a fertilizer.

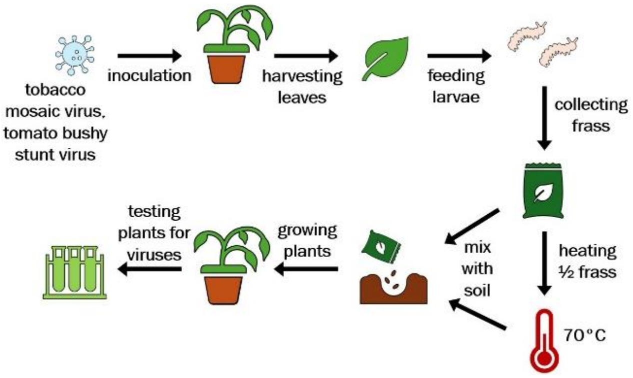

Figure 1. Project workflow – from plant inoculation with viruses and frass production, to growing the plants in the frass-substrate mixture and testing them.

Wastewater effluent shapes river viral communities

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Rivers are highly dynamic systems that provide critical habitat, resources, and movement corridors for wildlife, vegetation, and people. Viruses can survive and be transported within rivers as well, but little is known about how environmental factors, including human activities, shape the composition of riverine viral communities. Here, we investigated how wastewater effluent influences the dynamics of viral communities in its recipient river. We collected effluent samples from the wastewater treatment plant Domžale-Kamnik in central Slovenia monthly from April to October for two years. Concurrently, we sampled water from the effluent recipient river, Kamniška Bistrica, at three sites relative to the effluent discharge point: upstream, immediately downstream and several kilometres downstream. We characterized the viral communities of the effluent and river water by performing high-throughput sequencing of concentrated water samples and analysing the data with a custom bioinformatic pipeline. We showed that river viral communities were dominated by DNA bacteriophages and exhibited substantial month-to-month turnover. Despite this variability, we detected recurring annual patterns, with samples collected twelve months apart showing higher similarity in viral communities than those separated by six months. Viral community composition at the site upstream of the wastewater treatment plant consistently differed from both downstream sites throughout the sampling period, indicating that the wastewater discharge has a stronger influence on viral community structure than seasonal variation (Figure 1). Beyond the seasonal and wastewater-driven effects, we observed pronounced shifts in viral composition across all river sites during two non-consecutive months, October 2023 and July 2024. These shifts coincided with changes in river chemistry, but not with changes in the wastewater effluent, suggesting an unknown external disturbance of natural or anthropogenic origin. Overall, our results indicate that river viral communities are highly dynamic yet influenced by both seasonal and environmental changes, as well as external perturbations such as wastewater discharge.

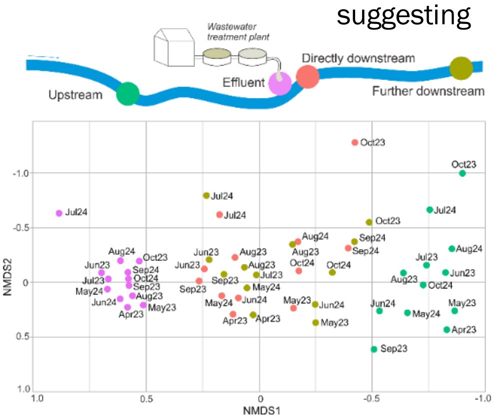

Figure 1. Virome composition of effluent influences downstream communities. Effluent = wastewater effluent. Upstream, directly downstream, further downstream = river sampling locations.

Comparison of different viral enrichment methods for compost virome analysis

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Compost is a nutrient rich organic fertilizer produced through the aerobic decomposition of various organic matter, such as food waste, plant residues and household waste. The process of composting itself might prove to be a better alternative for eco-friendly waste disposal, in comparison with anaerobic decomposition on landfills, because of the lower methane and carbon emissions. Although compost generally benefits crop production and the environment, it may also pose phytosanitary risks. Because compost contains large amounts of plant material, it may contain environmentally stable plant viruses that can persist outside their hosts and remain infectious. Their detection and characterization are technically challenging, due to the high levels of background nucleic acids and organic inhibitors, which can interfere with both reverse transcription quantitative PCR (RT-qPCR) and high-throughput sequencing (HTS) methods that are most often used for their detection. This is the reason why efficient enrichment of viral particles is a crucial step prior to downstream analyses. Here, our goal is to adapt and validate the most efficient enrichment protocol while comparing different concentration and purification approaches from studies done on similarly complex sample matrices (e.g. soil). Ultracentrifugation, ultrafiltration, flocculation and chromatography protocols are being tested and compared to improve the recovery of viral RNA, while reducing background nucleic acids originating from, e.g., bacteria, fungi and plants. The performance of these approaches is assessed using HTS analysis and RT-qPCR assays targeting spiked stable plant viruses, background bacterial, and fungal nucleic acids, where the best performing methods will be used for HTS analyses to investigate compost viromes using HTS. This work aims to contribute to a better understanding of compost as a potential reservoir of stable plant viruses and to support future studies on environmental plant virology.

Comprehensive investigation of direct piezoelectric response of $BiFeO_3$–$BaTiO_3$ ceramics using a custom-made dynamic Berlincourt press

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In this work, the piezoelectric properties of the (1–x)BFO–xBT solid solution, a promising piezoelectric material for sensor applications, were investigated [1]. In particular, we determined the direct longitudinal piezoelectric coefficient (d_{33}) and the tangent of the piezoelectric phase angle ($tan\delta_p$) in a frequency range between 90 Hz and 0.01 Hz, for different compositions around the morphotropic phase boundary (MPB), which is close to xBT =0.30. The irreversible (α) and reversible (d_{33}^{init}) Rayleigh coefficients were extracted for different frequencies [2]. These coefficients give an important insight in the extrinsic contributions, such as those arising from dynamics of domain walls, allowing a deeper comprehension of the compositionally dependent piezoelectric behavior of BFO-BT and thus the maximum response at MPB. Interestingly, such data are still not available for BFO-BT, primarily due the complexity of the experimental setup (Figure 1a and 1b). In this contribution, we will present the preliminary results obtained using our custom Berlincourt press setup, trying to highlight possible new direction in the studies of piezoelectricity in the promising BFO-BT ceramic system.

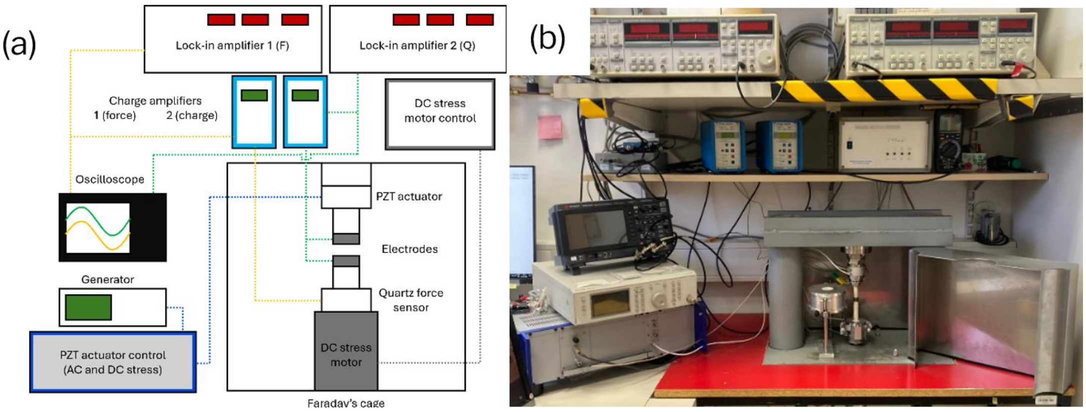

Figure 1. (a): schematic representation, and (b): picture of the setup. A motor applies the DC stress, while a PZT actuator applies the AC stress, regulated by a function generator. The signals of force (from a quartz sensor) and charge are amplified and sent to an oscilloscope and to two lock-in amplifiers.

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Preparation of polyimide thick films using powder aerosol deposition

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The preparation of polymer thick films remains challenging using conventional solvent-based, thermal, or vapor deposition methods, which are often limited to thickness control, use of solvent or high processing temperatures. In this work, we investigate powder aerosol deposition (PAD) – a room-temperature, solvent-free technique, traditionally used for the deposition of ceramic materials [1] – as a novel approach for fabricating pristine polyimide thick films. We examine how powder pre-treatment affects the particle size and morphology of the powder and, consequently, the deposition behavior, microstructural, mechanical and dielectric properties of PAD-deposited polyimide thick films. Commercially available polyimide powder was pre-treated by wet milling at 100 rpm, and dry milling at 100 rpm and 200 rpm, resulting in four different powders: raw, wet-100rpm, dry-100rpm, and dry-200rpm. PAD deposition was performed on gold-coated glass substrates under identical condition for all powders. As-prepared polyimide thick films were characterized from macroscopic to micro- and nanoscale using various techniques. Polyimide films from raw and wet-milled powders exhibit high deposition rates (up to 6.43 mm^3/min), thicknesses in the range of ten µm, dense and uniform homogeneous microstructures, and enhanced dielectric and mechanical properties ($\varepsilon_r \approx 8–9$, $\tan \delta < 0.017$, and $E \approx 3.30$ GPa). In contrast, films prepared from dry-milled powders showed inhomogeneous microstructures with voids and holes, low deposition rates, reduced dielectric permittivity ($\varepsilon_r \approx 4.0$), and lower Young's modulus. Differential scanning calorimetry and Fourier-transform infrared spectroscopy confirm that neither milling nor PAD itself alters the chemical structure of polyimide powders and films. These results demonstrate that optimized powder pre-treatment is critical for successful PAD of polymer thick films with tunable microstructural, mechanical, and dielectric properties, and opens new opportunities for applications in flexible electronics.

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Comparison of carbon-based screen-printed electrodes for detection of antibiotic sulfamethoxazole

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The increasing use of pharmaceuticals, especially antibiotics, has led to their accumulation in aquatic environments, where their high stability results in prolonged bacterial exposure to antibiotics and promotes the development of antibiotic resistance. Chromatographic techniques are commonly used for antibiotic detection; however, they are time-consuming, expensive and limited to laboratory use. In contrast, electrochemical techniques, particularly voltammetry, represent a promising alternative due to their fast analysis, low cost, and portability, especially when screen-printed electrodes are employed. (Figure 1) Sulfamethoxazole (SMX) is one of the most frequently used broad-spectrum antibiotics and is increasingly detected in aquatic environments, which highlights the need for fast, sensitive and selective detection methods. [1] This work presents a comparison of screen-printed electrodes (SPE) based on carbon materials. The electrodes investigated are SPE-C, with a carbon working electrode and SPE-SWCNT, with a working electrode modified with single-walled carbon nanotubes. Firstly, the supporting medium and pH were optimized. Then the electrochemical properties of the system were characterized, including the reversibility of the reaction, whether the process is diffusion- or adsorption-controlled and the active surface area of the electrodes was calculated. In addition, the background current and repeatability of both electrodes were evaluated. Finally, calibration curves were constructed and LODs of both electrodes were compared.

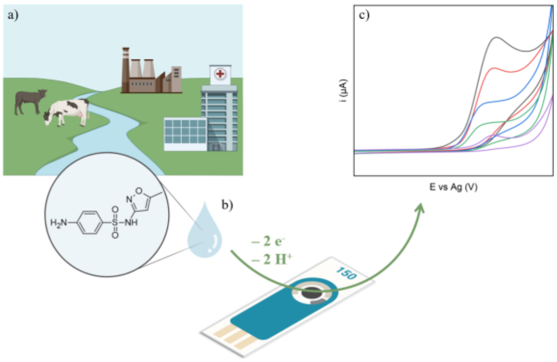

Figure 1. a) Sources of SMX residue in the environment, b) electrochemical detection and c) response to different SMX concentrations.

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Detection of genotoxic effects of xenobiotics using an advanced *in vitro* 3D hepatic cell model

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Body-foreign chemicals (xenobiotics) pose a substantial risk to human health due to their capacity to induce DNA damage, contributing to carcinogenesis and other chronic pathologies. Conventional 2D cell cultures and animal models often fail to reproduce human-specific metabolic processes, underscoring the need for more physiologically relevant *in vitro* systems. This study optimized and validated a dynamic three-dimensional (3D) HepG2-derived spheroid model for assessing genotoxicity and subsequently applied it to evaluate the effects of selected polycyclic aromatic hydrocarbons (PAHs) (Figure 1).

In the first experimental phase, spheroid development was characterized through analyses of growth, maturation, and metabolic activity. The spheroids demonstrated long-term stability and peak metabolic activity between days 17 and 22. Expression of hepatic markers (ALB, CK18, HNF4α) and induction of metabolic enzymes (CYP1A1, CYP3A4, NAT2, UGT1A1) confirmed functional maturation, leading to the selection of 21-day-old spheroids as the optimal model.

In the second phase, spheroids were exposed for 24 or 96 hours to benzo(g)perylene (BGP), benzo(b)fluoranthene (BBF), benzo(a)pyrene (BaP), or a BGP+BBF mixture. Flow cytometry revealed compound-specific genotoxic profiles, with increasing biomarker activation at higher concentrations. Overall genotoxic potency followed the order: BGP < BBF < BaP, with no synergistic effects observed in the mixture.

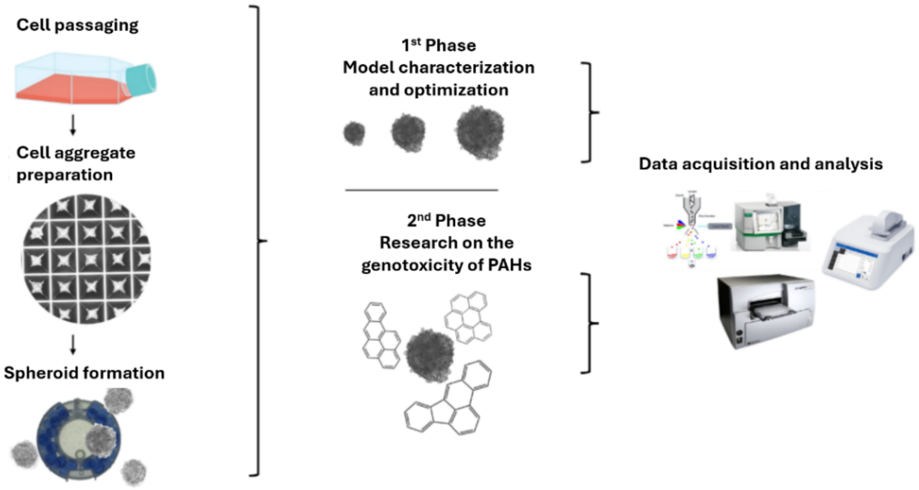

Figure 1. Experimental design of an in vitro 3D model used for assessment of PAH genotoxicity

Nanomaterials based genosensor with enzyme-assisted recycling amplification for pathogen identification

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Electrochemical biosensors have emerged as powerful analytical tools for the rapid, sensitive, and cost-effective detection of biological targets. Among them, electrochemical genosensors have gained significant attention due to their ability to selectively detect specific DNA and RNA sequences. These sensors typically rely on the hybridization between a target nucleic acid and a complementary probe immobilized on the electrode surface, converting this molecular recognition event into a measurable electrical signal. Owing to their high sensitivity, simple instrumentation, and compatibility with miniaturized platforms, electrochemical genosensors are widely explored for applications in medical diagnostics, environmental monitoring, and food safety [1], [2].

The detection of pathogen-related nucleic acids is particularly important for the early diagnosis and control of infectious diseases. By targeting unique genetic sequences from bacteria, viruses, or other microorganisms, genosensors enable highly specific pathogen identification [2]. In recent years, the use of enzyme-assisted signal amplification and nanomaterials has significantly improved the analytical performance of these systems [1].

In this work, the focus is on the synergistic integration of these strategies. Enzyme-assisted amplification will be based on enzymes, enabling selective process of nucleic acid structures formed during hybridization, generating amplified electrochemical signals and allowing detection of very low concentrations of DNA or RNA targets [3]. In addition, nanomaterials will be employed due to their excellent conductivity, large surface area, and strong affinity for thiol-modified DNA probes [1]. The combination provides an effective approach for the development of highly sensitive and reliable electrochemical genosensors for pathogen detection.

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Development of $Ni(OH)_2/NiOOH$–Polyaniline Electrochemical Sensors for Glucose Detection in Artificial Sweat

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Conventional glucose monitoring methods rely on invasive blood sampling, which is often associated with pain, discomfort, and psychological stress. Consequently, patient compliance is frequently inadequate, increasing the risk of severe complications. These limitations highlight the need for a non-invasive and reliable approach to continuous glucose monitoring. Sweat has emerged as a promising biofluid for wearable sensing applications due to its non-invasive accessibility, continuous production, and the presence of physiologically relevant metabolites, including glucose [1].

Non-enzymatic electrochemical sensors offer a robust alternative to commercial enzymatic sensors, providing improved stability, reproducibility, and resistance to environmental factors. Nickel hydroxide is a well-known electrocatalyst for non-enzymatic glucose detection, owing to its reversible Ni^{2+}/Ni^{3+} redox behavior, which facilitates efficient glucose oxidation. Furthermore, the addition of conductive polymers can improve electrical conductivity, electrocatalytic efficiency, and mechanical stability—key requirements for wearable sensing applications.

The first stage of the study focused on the electrodeposition of a conductive polymer (polyaniline) onto a gold screen-printed electrode. Key parameters, including potential window, aniline concentration, and scan rate, were systematically optimized using cyclic voltammetry to achieve a stable and uniform conductive film.

In the second stage, $Ni(OH)_2/NiOOH$ was deposited onto the prepared polymer-coated surface to develop the final electrochemical sensor. The fabricated electrodes were subsequently characterized to evaluate their surface morphology.

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Electrocatalytically enhanced nanobody-based electrochemical biosensor for prostate-specific antigen detection

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The identification and quantification of prostate cancer biomarkers are critical for early diagnosis and disease monitoring. Sensitive and selective analytical platforms are therefore required to detect these biomarkers in complex biological samples [1]. Despite significant advances in cancer diagnostics, there remains a need for rapid, high-performing, cost-effective, point-of-need, and accessible detection systems. Emerging electrochemical biosensing strategies aim to address these challenges by combining biological recognition elements with advanced functional materials.

In the present study, we synergistically combine a new class of electrocatalytic nanomaterials with nanobodies, as biorecognition elements, on the disposable screen-printed electrode system, for sensitive and selective detection of prostate-specific antigen (PSA). Nanobodies are single-domain antibodies derived from camelids [2]. Due to their small size, they allow for a higher surface density than antibodies and are oriented at the electrode surface via tag-mediated immobilization to ensure highly effective antigen binding. Future studies will aim to validate this biosensing strategy in real clinical samples and explore its potential for practical diagnostic applications.

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Hidden in the water: monitoring of avian influenza viruses in environmental waters

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Bird flu (avian influenza) is a top-priority zoonotic threat, posing significant global health and economic risks. It is caused by avian influenza viruses (AIVs), members of the *Alphainfluenzavirus influenzae* species, which infect a wide range of animal species — from birds to mammals, including humans — where they can cause severe illness and high mortality. Wild migratory birds are important vectors, transporting AIV over long distances and transmitting the virus to livestock and humans. Current surveillance mainly relies on sampling dead birds, which has several limitations. On the other hand, water-based epidemiology offers us surveillance on the population level. In this context, we explored environmental water monitoring for AIV surveillance.

We conducted a pilot monitoring study at two Slovenian lakes (Zbilje and Sestrže). At both lakes, grab samples were collected, and large volumes of water (50–70 L) were concentrated by ultrafiltration using a large-volume concentrator (LVC) combined with a concentration pipette (CP) (Innovaprep, USA). In parallel, torpedo passive samplers equipped with nylon or mixed cellulose ester (MCE) filters were deployed for eight days at Lake Zbilje. Nucleic acids were extracted and tested for Influenza A virus and the H5 subtype using RT-qPCR (Figure 1).

Over nearly two years of monitoring, multiple samples were positive for the influenza A virus, including the H5 subtype. Torpedo samplers proved to be a simple and cost-effective alternative to grab sampling with ultrafiltration. Environmental water monitoring may therefore allow us to research across borders of existing surveillance strategies and support early detection and preparedness for future avian influenza outbreaks.

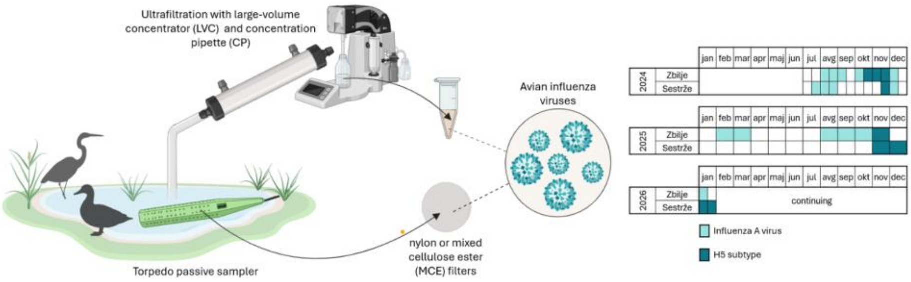

Figure 1. Monitoring of avian influenza virus in the lake and monitoring results (Created with BioRender.com). Coloured rectangles represent positive detections.

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