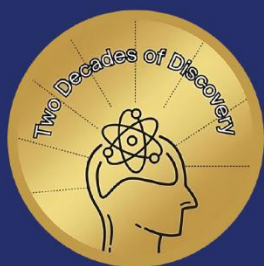


# Two Decades of Discovery: Advancing Science and Solutions.



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16th Jožef Stefan International Postgraduate  
School Students' Conference



*16th Jožef Stefan International  
Postgraduate School Students' Conference*

*Book of abstracts*

*Edited by:*

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## IPS Student Council

This year, the Jožef Stefan International Postgraduate School (IPS) celebrates its 20<sup>th</sup> anniversary. To celebrate this milestone, the chosen theme for the 16<sup>th</sup> edition of the IPS Student Conference (IPSSC 2024) is **“Two Decades of Discovery: Advancing Science and Solutions.”** Over the past two years, the conference was set in the lovely, cozy town of Kamnik. However, for this year’s celebration, we decided to switch to the sunny, exciting Piran, which offers a vibrant and picturesque backdrop for this year’s milestone event; therefore, we chose the National Institute of Biology’s Marine Biology Station to hold the important and engaging scientific discussions of IPSSC 2024.

To mark two decades of IPS, numerous alumni were invited to showcase how the school has influenced their development and career preparation. The conference featured a varied program with lectures from the invited alumni. These included talks by invited speakers such as “Nanomedicine” by Dr. Nina Kostevšek from the Jožef Stefan Institute (JSI), and “Infinite - From Scientific Curiosity to New Disruptive Technology on the Health-Hazard Assessment Market” by Dr. Janez Štrancar from Infinite and JSI.

A round table about exploring career options and how IPS has influenced their career paths was also held with alumni of the IPS. This included Dr. Kristina Žagar Soderžnik from JSI, Dr. Blaž Fortuna from Extrakt.AI, and Dr. Jelena Isailović from the National Institute of Chemistry, who shared their professional and personal experiences during and after their PhD journeys. Dr. Rok Novak gave an exciting lecture about his PhD and life after it in his talk “Stumbling into Academia.” The alumni presentations not only highlighted the diverse career paths taken by our graduates but also served as an inspiration for current students, showcasing the real-world applications of the knowledge and skills honed at IPS.

In addition to the IPS Alumni, we counted on the expertise of Mlada Akademija, represented by Mateja Erce Paoli and Dr. Ana Slavec, to discuss challenges faced by researchers with the talk “Researcher Mental Health”.

IPSSC 2024 welcomed approximately 63 participants who contributed to the outstanding collection of abstracts, posters, and presentations on various interesting topics, which are presented in the proceedings and will stimulate further discussions. It is inspiring to witness the tremendous effort put into advancing science while solving today's and tomorrow's societal problems through science. This conference provides a rare opportunity to meet and engage with people who share similar fields of interest, offering a great potential for future cooperation. The insights shared and connections made here not only celebrate our past achievements but also pave the way for innovative solutions to emerge.

We are profoundly grateful to all the students, invited speakers, professors, mentors, members of the scientific committee, and the Dean of IPS, Prof. Milena Horvat, as well as the dedicated IPS team consisting of Dr. Aleksander Zidanšek, Sergeja Vogrinčič, Maša Matijašević, and Tadeja Samec. We extend our thanks to our sponsors IPS, Jožef Stefan Institute, National Institute of Biology, Ljubljana University Incubator, Trimo, BSH Hišni aparati, Gorenje, Alpacem, National Institute of Chemistry, Avantor, Kolektor, Generali, Luka Koper, Premogovnik Velenje, Red Bull, Leone, and Sanolabor for their support in making this conference free of charge for all participants. And last but not least, we sincerely thank the exceptional organizing team for making the conference happen.





As we reflect on the success of IPSSC 2024, we are reminded of the power of collaboration and the exchange of knowledge. We eagerly anticipate the advancements and community growth this conference will inspire.

Thank you all, and we look forward to seeing you next year!

Alnilan Lobato and Mark Zver,

on behalf of the IPS Organizing Committee and the IPS Student Council

## 20 years of partnership and progress: commemorating JSIPS and student success

It is with immense pride and joy that we come together to celebrate the 20th anniversary of the Jožef Stefan International Postgraduate School (JSIPS). Over the past two decades, JSIPS has evolved into a center of excellence, fostering innovation and academic achievement. This success is largely due to the engagement and empowerment of our students, as well as the strong collaborations with our founding institutions, including the Jožef Stefan Institute, the National Institute of Biology, and the Institute for Metals and Technology, along with our industrial partners. This milestone not only commemorates our history but also stands as a testament to the dedication and hard work of our students, faculty, and staff.



The IPS Student Conferences have become a celebrated tradition and one of the most significant annual events for our school. This year's conference marks the 16th gathering with the theme, **"Two Decades of Discovery: Advancing Science and Solutions"**. This theme reflects the high-tech demands and rapid technological advancements of today's world. The variety of topics covered in this conference underscores our students' responsiveness to contemporary societal trends and needs, demonstrating their ambition and commitment, even at this early stage of their research and development careers.

One of the key strengths of these conferences is the emphasis on clear and understandable communication of research results. This process is most effective when excellence, creativity, and innovation are evident in the scientific work presented. An in-person conference provides an invaluable opportunity to strengthen cooperation within and between different scientific disciplines of the IPS study program and beyond, including various sectors of society.

This year, we are particularly honoured to organize the conference at the National Institute of Biology's Marine Biological Station in Piran. This small coastal area of Slovenia is a national treasure, often referred to as a pearl due to its breath-taking beauty. The sea has imparted a magical quality to our conference, and many of us have found inspiration in the expansive views of the horizon. There is a symbolic resonance in holding our conference here, as the endless possibilities of the open sea mirror the boundless potential of scientific discovery.

The organization of this year's IPS conference has been a demanding task, entirely managed by the Organizing Committee and the IPS Student Council. JSIPS and its partners are extremely proud of their commitment and excellent organization. Congratulations to all who were responsible for the organization and to those who registered for the conference!

Special thanks also go to the sponsors of the IPS Conference. Your moral support and recognition mean more than financial contributions. Additionally, we must not forget the mentors who guide our students and help them achieve their ambitious goals. Recognition goes to everyone—students, mentors, JSI support staff, partners, and founders of the school.

It is with profound admiration and gratitude that we commemorate the 20th anniversary of JSIPS. This journey of academic excellence and innovation has been a visionary undertaking, led by the determined spirit of figures like President of the JSIPS Prof. Dr. Vito Turk and the late Prof. Dr. Robert Blinc. Their foresight and dedication laid the foundation for what JSIPS has become - a guiding light of intellectual pursuit and scholarly achievement.

*Furthermore, we recognize the potential for further integration of our Alumni Club into the academic life of JSIPS. With over 530 PhDs and over a hundred master's degree holders among our alumni, they represent a vast repository of knowledge and experience. However, the Alumni Club is still in the process of defining its role, seeking to become more engaging and relevant to current JSIPS students. By leveraging the expertise and insights of our alumni, we can enrich the academic experience, fostering stronger connections between past and present students, and providing valuable resources for future endeavours. Ultimately, while quality remains our primary goal, we understand that true enrichment comes from individuals who take on responsibilities and work for the advancement of society. As we strive for academic excellence, let us also cultivate a culture of responsibility and service, ensuring that our contributions extend beyond the school's boundaries and positively impact society as a whole.*

As we gather to celebrate this milestone, let us honour the legacy of those who paved the way for us while committing ourselves to the pursuit of excellence and innovation that defines JSIPS. Together, let's embark on the next chapter of our journey, guided by the principles of curiosity, collaboration, and persistent pursuit of knowledge.



Prof. Dr. Milena Horvat

Dean JSIPS

# Ecotechnologies

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

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This study investigates strategies to enhance the efficiency of biophotorelectrochemical (BPEC) processes through the structured formation of biofilms comprised of aerobic phototrophic microorganisms. By harnessing the photosynthetic capabilities of microalgae and cyanobacteria, BPEC systems combine bioelectrochemistry and photoelectrochemistry to catalyse redox reactions driven by light energy. The reviewed literature focuses on the development and characterization of artificial biofilms, utilizing polyelectrolytes to immobilize microorganisms on electrode surfaces. Analytical techniques, including cyclic or linear voltammetry and microscopic imaging, have been employed by various researchers to assess the electrochemical performance and morphology of biofilms. Their results demonstrate that structured biofilms exhibit enhanced power output and stability compared to natural biofilms, with significant improvements observed in current generation and substrate reduction capabilities. These findings underscore the potential of biofilm structuring as a promising approach to optimize BPEC systems for various renewable energy and environmental applications. Preliminary findings of our research demonstrate successful attachment of the microalgae *Chlorella sorokiniana* to regular and conductive glass substrates using polyethyleneimine (PEI) polymer. Like in reviewed literature, we will analyse the biofilm by microscopic and voltametric analysis to optimize the biofilm structuring method. In further research we aim to test novel electrode materials, various polyelectrolytes, and cyanobacterial strains to advance the development of sustainable and efficient BPEC technologies.

## Cluster analysis of *tert*-butyl dimethyl silyl (TBDMS) derivatives dataset

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In the field of environment and health studies, the identification of contaminants of emerging concern (CEC) has recently received increased attention. For this complex and challenging task, resources, such as compound databases (DBs) and mass spectral libraries (MSLs) concerning these compounds are sorely needed. This is especially the case for semi polar organic contaminants that have to be derivatized prior to gas chromatography-mass spectrometry (GC-MS) analysis with electron impact ionization (EI). Recently, Ljoncheva et al. have constructed and made publicly available several datasets of GC-EI-MS spectra, including a dataset of MS of *tert*-butyldimethylsilyl (TBDMS) derivatives, containing mass spectra acquired by the authors, as well as metadata about the chemicals, including their structures (e.g., InChiKeys and SMILES codes).

We perform exploratory data analysis of the TBDMS dataset, performing clustering to identify groups of chemicals which are similar. The clustering method used will be that of predictive clustering trees. The clustering will be performed according to a distance based on the spectral information. In particular, the mass spectra will be transformed using the Spec2Vec approach to produce feature vectors, on which the Euclidean distance will be applied.

We will inspect and comment on the identified clusters. For the clusters, which will be based on the similarity of mass spectra, predictive clustering trees will provide explanations in terms of structural features from a given set of molecular fingerprints (and their combinations): we will analyse and comment on the structural features of the chemicals that cluster together. We will finally discuss directions for further work to exploit this unique, but so far underused dataset.

## Size-dependent bacterial distribution and correlation with mercury concentrations

**Tamara Kerševan**<sup>1\*</sup>, Igor Živković<sup>2</sup>, Tomaž Rijavec<sup>2</sup>, Jože Kotnik<sup>2</sup>, Aleš Lapanje<sup>2</sup>, Milena Horvat<sup>2</sup>

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The aim is to explore the interplay between the development of bacterial communities and the size of suspended particles in freshwater samples. The focus is on unravelling bacterial natural distribution and abundance along seven size fractions and their relationship dependent on the particles present.

Particle size influences the surface area for bacterial colonisation as increased surface area can promote bacterial growth and activity. Particle size also influences the dispersion in aquatic environments – the size of particles to which bacteria attach can dictate the dispersal patterns in the water column. Furthermore, particle surfaces serve as attachment sites for bacterial biofilm formation and their size dictates the complexity and stability of biofilms.

The study investigates bacterial distribution in the Idrija river, which is marked by the presence of mercury. In the Idrija valley, mercury occurs both naturally and from past industrial activities like smelting. For that reason, the research expands beyond bacterial characterisation, seeking to understand the impact of the pollutant on the bacterial communities, with a specific focus on understanding size-dependent dynamics.

Size fractions (ranging from 0.2 to 180.0 micrometres) are obtained by filtering the water samples, and DNA is isolated. Subsequent polymerase chain reaction (PCR) amplification and sequencing facilitate the targeted assessment of the genetic information in the microbial communities. By measuring the concentrations of mercury (and methylmercury) in each size fraction, we expect to reveal size-specific adaptations and preferences of bacteria in response to varying pollutant levels as well as identify possible bioaccumulation patterns.

The unique focus on size-dependent dynamics provides novel insight into the bacterial communities in polluted environments, where implications of the research could extend to the realm of bioremediation. Furthermore, the established method could be also applied to soil, sediments, and environments with other pollutants present.

## Are Surface-Active Substances Influencing the Particle Dynamics?

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Surface-active substances (SAS), commonly found in atmospheric aerosols, exist at the interface of atmospheric particles, and have a significant impact on various atmospheric phenomena, including cloud condensation nuclei (CCN), ice nucleation, multiphase and photochemical reactions [1]. Their presence may enhance the adsorption or uptake of more hydrophobic compounds onto particle surfaces, potentially affecting their interface chemistry and the growth of newly formed particles [2].

The change in surface tension caused by the presence of SAS in bulk samples can be studied using various dynamic and static methods, such as the Wilhelm plate, de Nouy tensiometer, oscillating bubble tensiometer, axisymmetric pendant drop tensiometer and the ring-down tensiometer [1]. However, due to their sensitivity to salinity, they are unsuitable for quantifying the physical properties of SAS present in atmospheric particles.

For this reason, inspired by previously overlooked literature, our study presents an innovative interpretation of an electrochemical technique, called electrochemical tensiometry. This method quantifies the reduction of surface tension in atmospheric aerosol particles caused by SAS. We demonstrate its utility in studying gas uptake and the influence of SAS on the particle growth process.

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- [1] V. F. McNeill, N. Sareen, and A. N. Schwier, *Topics in Current Chemistry*. **2013**, 339, 201-59.
- [2] B. T. Mmereki, D. J. Donaldson, *Phys. Chem. Chem. Phys.* **2002**, 4, 4186–4191.

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## Synthesis of inorganic compounds of some metals with XeF<sub>2</sub> and their characterization

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In 1962, the first compound with a noble gas, XePtF<sub>6</sub>, was synthesized. Since then, numerous others have been made. Among them, XeF<sub>2</sub> has been the most extensively researched. It functions as a good fluorinating and oxidizing agent. In my doctoral thesis, I focus on synthesizing coordination compounds where XeF<sub>2</sub> is bound as a ligand to a metal ion, following the general formula [M<sup>n+</sup>(XeF<sub>2</sub>)<sub>p</sub>](AF<sub>6</sub>)<sub>n</sub> (M is a metal in oxidation state n, A=As, Sb, Bi, P, Ta, Ru, etc.) [1]. Compounds of this kind are typically prepared through the reaction between M<sup>n+</sup>(AF<sub>6</sub>)<sub>n</sub> and XeF<sub>2</sub>, where XeF<sub>2</sub> can be in excess or in stoichiometric quantity, or through direct synthesis involving MF<sub>n</sub>, XeF<sub>2</sub>, and PF<sub>5</sub> or BF<sub>3</sub>. In my doctoral research, I will attempt to introduce novel synthetic routes, such as the reaction between [XeF<sup>+</sup>][AF<sub>6</sub><sup>-</sup>] or [Xe<sub>2</sub>F<sub>3</sub><sup>+</sup>][AF<sub>6</sub><sup>-</sup>] and MF<sub>2</sub>. Reactions are conducted in specialized reaction vessels constructed from fluorinated polymers and equipped with Teflon valves. I use anhydrous HF as the solvent, and due to reactant sensitivity to moisture, I weigh and add them inside reaction vessel in a glove box. Crystallization of the product is performed in specialized vessels. Coordination compounds are initially characterized using Raman spectroscopy, with the typical XeF<sub>2</sub> peak at 497 cm<sup>-1</sup>, shifting to higher values when XeF<sub>2</sub> is bound to the metal ion. Single-crystal X-ray diffraction provides a detailed view of the coordination compounds' composition. My goal is to synthesize and characterize as many coordination compounds of this type as possible [2].

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## Removal of bisphenols from drinking and waste- water using hydrodynamic cavitation and photocatalysis

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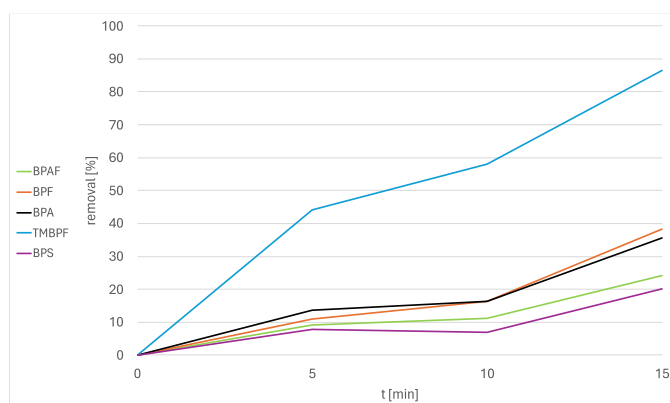
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The global demand for freshwater for industrial, agricultural, and domestic purposes continues to increase, affecting the quantity and quality of freshwater sources, many of which represent important sources of drinking water. One possible solution to this problem is using treated wastewater in industry and agriculture. However, such replacement poses numerous challenges as wastewater is a major source of contaminants of emerging concern (CECs), including endocrine-disrupting compounds such as bisphenol A (BPA) and its substitutes. Unfortunately, conventional wastewater treatment technologies are not optimised to remove CECs, creating a need for additional treatment technologies, such as advanced oxidation processes (AOP).

In this study, the removal of BPA, bisphenol S (BPS), bisphenol F (BPF), bisphenol AF (BPAF) and tetramethyl bisphenol F (TMBPF) from drinking and treated wastewater using hydrodynamic cavitation and photocatalysis was investigated. For this, known amounts of bisphenols were spiked into drinking water (200 ng/L) and treated wastewater (1.0 µg/L), and then subjected to cavitation and photocatalysis separately, sequentially, or simultaneously. During the experiment, samples were collected at determined time intervals, extracted using solid-phase extraction, derivatised and then analysed using gas chromatography-mass spectrometry (GC-MS). Notably, combining photocatalysis and cavitation resulted in the highest removal of bisphenols, i.e., 24–86% in drinking water and 4–19% in treated wastewater (Figure 1).



**Figure 1.** Removal of BPA, BPS, BPF, BPAF and TMBPF with time from drinking water treated simultaneously with hydrodynamic cavitation and photocatalysis.

## Advancing Seafood Authentication: Integrated Isotope and Elemental Techniques for Origin and Production Method Verification

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Fish and seafood are among the most vulnerable products to food fraud due to their complex supply chains, high value, and susceptibility to substitution and mislabelling. Consumers are increasingly interested in detailed information about the species, production methods, and geographical origins of their food. Thus, dealing with fraud is becoming more and more important.

The aim of this study is to establish an appropriate authenticity and traceability system for fish and seafood to verify the origin and production (wild vs. aquaculture) using stable isotope ratios of light elements (expressed as  $\delta^{13}\text{C}$ ,  $\delta^{15}\text{N}$ ,  $\delta^{34}\text{S}$ ,  $\delta^{18}\text{O}$ ), elemental composition, and multivariable statistical models. Two hundred samples of fish and mussels were collected from the Mediterranean Sea and the Atlantic Ocean, during the summer and autumn of 2023. Sample collection consisted of aquaculture Seabass and Seabream, wild Seabream and mussels. Stable isotope composition of C, N and S was determined by elemental analyzer coupled to isotope ratio mass spectrometer (EA-IRMS) in the lyophilized and defatted fish fillets and edible parts of mussels, while  $\delta^{18}\text{O}$  values were obtained in water squeezed out of fish samples. The  $\delta^{18}\text{O}$  values were determined by a Multiflow system connected to IRMS. Furthermore, the multi-elemental composition of 30 elements (Li, B, Na, Mg, P, S, K, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Rb, Sr, Mo, Ag, Cd, Sn, Sb, Ba, Hg, Tl, Pb, U) was simultaneously performed in the lyophilized samples through Inductively Coupled Plasma Mass Spectrometry (ICP-MS). We expect that the formulated diets and the pond's natural productivity of farmed seabass will mean that farmed fish will have significantly different isotopic and elemental signatures compared to wild animals.

The developed methodology in this study, supported by a literature-based database, will provide a sound basis for establishing an adequate traceability system for fish and seafood.

### Acknowledgments:

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## Effects of Fluoride, Aluminium and Their Complexes on Macrophage Viability In Vitro

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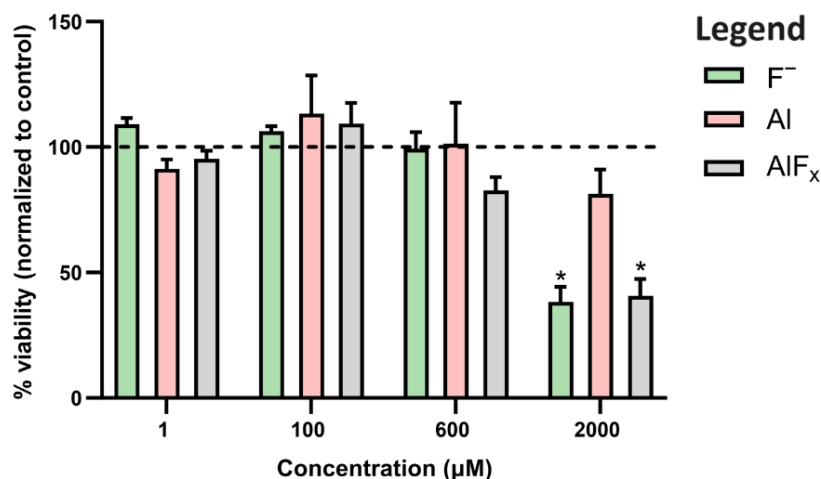
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Both fluoride and aluminium have been shown to have toxic and immunomodulatory effects on immune cells, especially macrophages [1,2]. In addition, aluminium fluoride complexes (AlF<sub>x</sub>), which can easily form in the environment, are known to alter the phosphorylation state of proteins through G-protein mimicry [3]. The theoretical mechanism of AlF<sub>x</sub> toxicity is well described, but there is a critical lack of *in vitro* studies investigating the toxicity of this species. The aim of our study was to investigate and compare the toxicity of fluoride (F<sup>-</sup>), aluminium (Al) and their complexes using a macrophage *in vitro* model. The viability of the macrophages was assessed using the PrestoBlue assay, in which metabolically active and therefore viable cells convert resazurin dye into fluorescent resorufin. Macrophages were exposed to standard F<sup>-</sup>, Al or AlF<sub>x</sub> solutions (1–2000 μM) for 48 hours, stained and the resulting fluorescence was quantified using a Cytation 5 microplate reader (BioTek, USA). Our results show (Figure 1) that at lower concentrations (1 μM, 100 μM), the F<sup>-</sup>, Al and AlF<sub>x</sub> species slightly increase cell viability compared to the negative control. However, at higher concentrations (600 μM, 2000 μM), cell viability decreases noticeably. Our results suggest, that the AlF<sub>x</sub> species pose the highest toxicity to macrophages among the studied species, triggering significant decrease in cell viability at higher concentrations.



**Figure 1.** Reduction of PrestoBlue reagent as a correlate of cell viability after stimulation with F<sup>-</sup>, Al and AlF<sub>x</sub> standards. Values are normalized to the control group (indicated by the dotted line) and shown as means with standard errors. (\*) indicates statistically significant differences with negative control

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## Exploring ways of removing PFAS from wastewater: Application of Cold Atmospheric Plasma

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Per- and poly-fluoroalkyl substances (PFAS) are a class of synthetic chemicals known for their unique properties, including resistance to heat, water, and oil, making them useful in a wide range of industrial and consumer applications, such as non-stick cookware, firefighting foams, and waterproofing materials. Due to their persistence in the environment, they are also termed 'forever chemicals' and have been shown to have toxic effects on environmental organisms and humans when exposed at low levels, causing liver damage, thyroid disease, fertility issues, and cancer.

Wastewater from industrial discharges, municipal sewage, and runoff from areas where PFAS-containing products are used or disposed of are major sources of PFAS in the aquatic environment. Their recalcitrance and continuous input pose significant challenges for water quality management and environmental conservation efforts. Because of this, various removal technologies are being investigated based on physical, chemical, and biological processes.

My research will focus on atmospheric pressure plasma as a promising technology for wastewater treatment (Fig. 1). This innovative technology uses high-energy plasma discharge to generate reactive species capable of degrading PFAS. Emphasis will also be on developing a robust analytical method for quantifying these contaminants in various aqueous matrices and identifying sources of uncertainty to ensure the reliability of analytical results, aiding in informed decision-making processes.

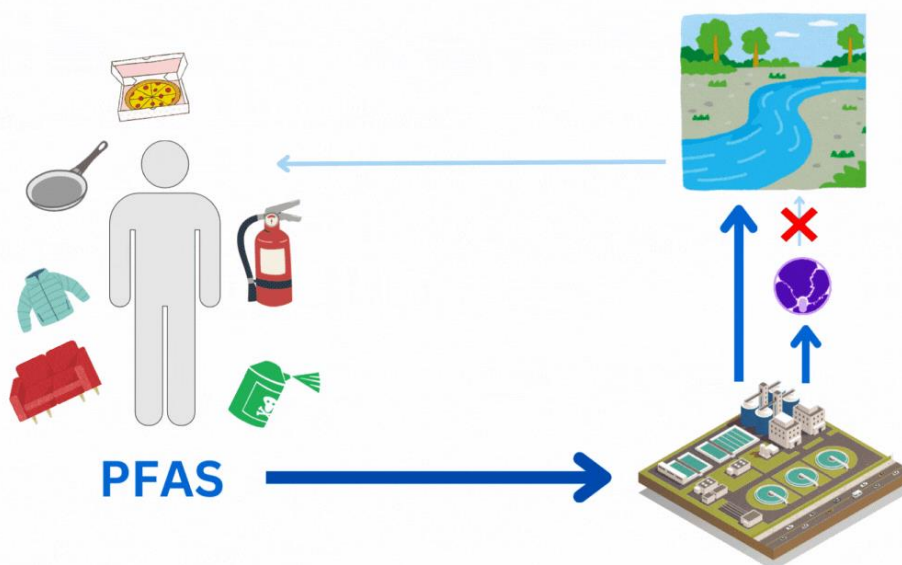


Fig 1: Advanced wastewater treatment: removing PFAS with atmospheric pressure plasma

## Toxicity of Bisphenol A, its analogues Bisphenol AP and Bisphenol C and their binary mixtures

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Bisphenol A (BPA) is one of the most used chemicals in industrial production of synthetic polymers, most notably in polycarbonate plastics and epoxy resins. Due to its versatility in industrial applications and use in numerous everyday products, its presence in environment is ubiquitous. Concerns about BPA's hazard on human health have increased over the last two decades, leading to regulatory restrictions and development of its analogues that are presumably safer alternatives. Analogues are gradually replacing BPA, although our knowledge on their toxicological profile and combined effects is limited. Here, we investigated the toxic effects of BPA and its analogues Bisphenol AP (BPAP) and Bisphenol C (BPC) and their binary mixtures (BPA+BPAP and BPA+BPC) on spheroids developed from human hepatocellular carcinoma (HepG2) cells. Cytotoxicity, genotoxicity, and expression of selected genes involved in DNA damage response and xenobiotic metabolism were examined after the exposure to single BPs and binary mixtures at 10, 20, 40, 10+10 and 20+20  $\mu\text{M}$  for 24 h, and 1, 2, 4, 1+1 and 2+2  $\mu\text{M}$  for 96 h. BPA did not reduce cell viability (MTS assay) in HepG2 spheroids after both exposure times, conversely BPAP and BPC affected cell viability at the highest concentration tested. Genotoxicity was assessed by the comet assay, which indicated that all BPs and binary mixtures resulted in elevated DNA strand break formation after 24 and 96 hours of exposure. BPC exhibited the highest genotoxic potential, causing DNA lesions at  $\geq 10 \mu\text{M}$  (24h) and  $1 \mu\text{M}$  (96h). No combined DNA damaging effects due to exposure to binary mixtures were observed. BPs and both binary mixtures upregulated (qPCR) the expression of genes involved in xenobiotic metabolism. Our results contribute new knowledge on the toxicity of BPA analogues and their complex mixtures; however, further research is needed due to their increasing production and development.

### Acknowledgments:

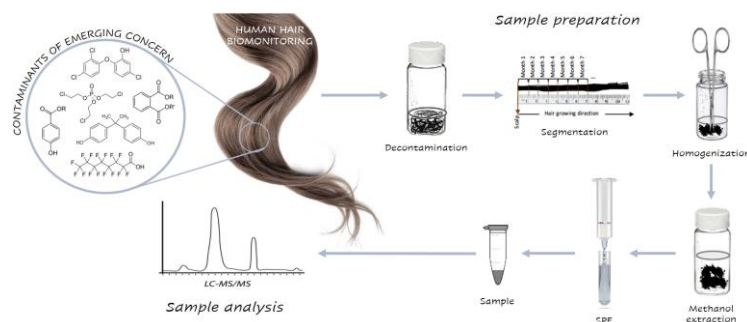
Supported by ARIS [P1-0245, J1-2465, Z1-3191], bilateral projects between Slovenia and Croatia [BI-HR/18-19-003; BI-HR/20-21-019], by the University of Zagreb, by the European Regional Development Fund project Farmlnova (KK.01.1.1.02.0021) and European Union HE project CutCancer; 101079113).

## Determination of contaminants of emerging concern in hair as a complementary matrix for human biomonitoring

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**Figure 1:** Workflow of hair analysis.

Human biomonitoring studies are important tools in scientific research, providing crucial insights into human exposure to environmental contaminants and their potential health effects. The monitoring of contaminants is performed by measuring the relevant exposure biomarkers in biological matrices, such as blood, and urine, and less used matrices such as hair, nails, saliva, and deciduous teeth. In this seminar, I will be addressing the topic of hair as a matrix for contaminant analysis. Historically hair was mostly used for the detection of toxic metals, pharmaceuticals, and drugs of abuse. However, more recently, it has been employed in the biomonitoring of exposure to organic contaminants.

Many chemicals pose a potential risk to human health and the environment, yet some remain unregulated by existing environmental laws. These substances, known as contaminants of emerging concern (CECs), are also the focus of this seminar. Developing new techniques for the determination of CECs involves designing new analytical methods for their extraction, annotation, and quantification from hair samples. This process involves the review and evaluation of existing procedures and upgrading them for optimal determination of CECs of interest. Usually, methods are developed for only one chemical or specific class, but lately, many authors have been determining many xenobiotics in the hair simultaneously.

Hair matrix is famous for its non-invasive sample collection, sample stability, and ease of storage. Furthermore, the possibility of segmental analysis of the hair matrix offers a unique way to detect contaminants, each segment representing a specific timeframe for exposure. However, analysis of hair comes with specific challenges such as external deposition of contaminants on the hair surface and optimization of decontamination procedures. Additionally, interpretation of results is difficult due to interindividual variability in absorption and metabolism of xenobiotics and because of different hair colors related to the melanin content and hair treatments.

## The purpose of participatory research in urban health

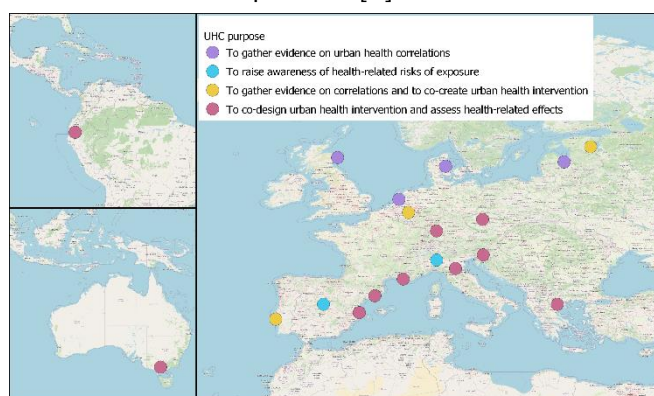
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Research and practice of the interface between urban environments and human health is broadly known as urban health. The use of participatory approaches in urban health is becoming paramount to harness the relationship between researchers, government, industry, and civil society. However, the effectiveness of participatory methods has been rarely reported in the scientific literature [1]. This study aims to establish a state-of-the-art around participatory methodologies used in urban health research by reviewing the Urban Health Cluster pilot studies funded under the Horizon 2020 European Programme. Following a convergent mixed-methods approach, this study reviewed 20 pilot studies. First, pilot cities completed an online written survey. Then, 3 project leads participated in semi-structured interviews to expand in more details. Both, the pilot city-level survey and semi-structured interviews aimed to characterize the purpose of using participatory methods, mechanisms of participation, expected outcomes, evaluation strategies, and challenges. Preliminary findings indicate the predominant purpose for including participatory methodologies is to co-design urban health interventions and assess health-related effects (Figure 1). This suggests that urban health research is developing context-specific interventions and producing evidence on the causal relationships between urban environment and human health outcomes. However, the results regarding the expected outcomes and evaluation strategies suggest the lack of a theory of change describing the potential participatory-led urban health transformation. Future steps include the application of frameworks (e.g., behaviour change theories) for the systematic and reproducible deployment and evaluation of participatory approaches in urban health research and practice [2].



**Figure 1.** Pilot cities from the Urban Health Cluster (UHC) and their purpose for including a participatory approach.

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## Using exposure load to examine the burden of multiple chemicals in men and lactating women

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The Exposure Load or EL is a semi-quantitative metric for evaluating multi-chemical exposure representing the number of chemicals with the measured concentration exceeding a given threshold, either the limit of detection or quantification (LOD or LOQ) or a certain percentile. It was first used on the data from the Canadian Health Measurement Survey and the results published in 2021. This study utilizes the exposure load to evaluate the results of the first Slovene Human Biomonitoring programme (HBMI), performed between 2007 and 2015. The sample consisted of 1098 men and lactating primiparous women aged between 18 and 49 from 12 areas, categorised as urban, rural or contaminated. The EL values were compiled using measurements for 30 chemicals belonging to elements, PAHs, phthalates and bisphenols at the 50<sup>th</sup> and the 90<sup>th</sup> percentile, while the EL at the LOQ also included 30 POPs, bringing the number of chemicals to 60. To reduce the impact of missing data and to account for differences in exposure routes for different chemicals, both total and partial ELs for each chemical group were calculated. In the statistical analysis, biserial correlation between the EL values and the individual chemicals was first calculated. The ELs were afterwards tested for differences between areas and area categories, sex, age groups and smoking status using non-parametric tests. Lastly, Poisson regression was performed for the ELs and the data collected through surveys, first bivariate and then multivariate based on the results of the former in an attempt to create predictive models. Most prominent determinants linked with higher EL urban areas at all thresholds, smoking status and male sex at higher thresholds, high BMI for PAH and phthalate EL and high seafood intake for element EL. Three multiple regression models with an adequate fit were also created. The metric holds promise for future practical use.

## Enhancing Bioleaching Efficiency for Metal Recovery from WEEE

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Bioleaching is an extraction process, besides pyrometallurgy and hydrometallurgy, which employs microorganisms for extraction of metals from various materials, such as electronic waste, municipal waste, red mud, mine tailings, low-grade ores, etc. The most commonly used microorganisms in bioleaching are *Acidithiobacillus ferrooxidans* and *Acidithiobacillus thiooxidans*. In bioleaching, microorganisms interact with metal particles, converting them into dissolved species through various reactions (Figure 1). Factors such as pH, temperature, pulp density, bacterial growth, and particle size influence the process [1]. My research focuses on waste electrical and electronic equipment (WEEE). Globally, 50 million tons are generated annually, with 4.7 million tons in the EU alone. Commonly recovered metals through bioleaching include Cu, Ni, Zn, and Co [2]. The aim of this work is to use and improve bioleaching to achieve best possible recovery of valuable critical raw materials from electronic waste, and to compare this method to pyrometallurgy and hydrometallurgy, also from economic and environmental point of view.

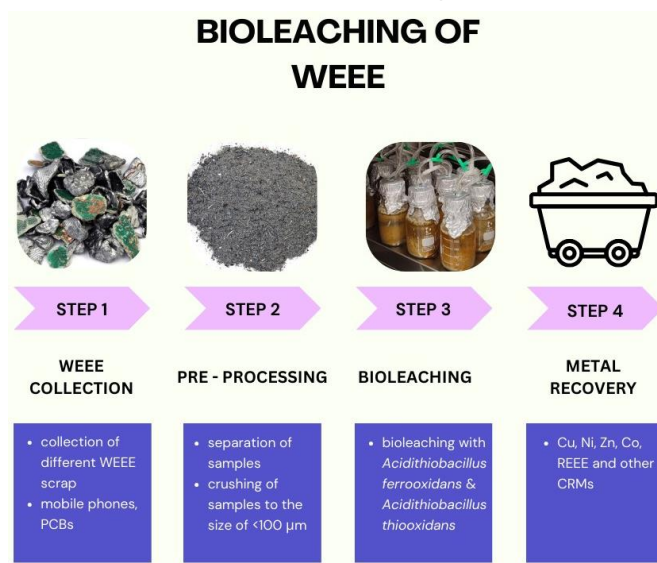


Figure 1. Process of WEEE bioleaching

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# Artificial Aggregates from Fly Ash for a Sustainable Build Environment

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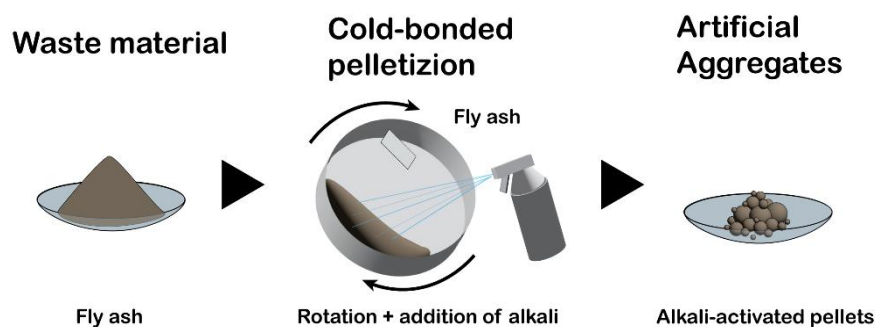
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Natural aggregates, essential materials for construction composites like concrete and asphalt, are the world's most extracted materials, usually through energy-intensive processes like mining or crushing. Representing 60-80% of the volume of concrete, aggregates represent one of the potential key areas of research for a sustainable build environment.

Therefore, this research proposes a sustainable alternative using biomass fly ash, a coal combustion byproduct, to produce artificial aggregates (AA). Despite the high calcium content of used biomass fly ash, which is typically unsuitable for cement, its significant silicon (Si) and aluminium (Al) content in the amorphous phase makes it suitable for producing alkali-activated aggregates when mixed with an alkali solution. Three batches of AA were produced using a disc pelletizer, varying the alkali solution and using only water as a control (Figure 1). Following cold-bonding palletization, AA samples were subjected to two different curing conditions, ambient and elevated temperature with higher humidity, to study the mechanical property evolution over time. The influence of the mixture design and curing on the AA was investigated with mechanical testing, Hg porosimetry, SEM, XRF and XRD to evaluate changes in chemical properties, mechanical strength and microstructure. The batch with the highest alkali solution content exhibited superior compressive strength due to a Si/Al molar ratio close to the theoretical ideal. Lower alkali solution mixtures exhibited reduced strength and efflorescence due to sub-optimal ratios and higher water content. Water-only mixtures had the weakest mechanical properties. However, curing at elevated temperatures and humidity (40 °C, 80 RH%) significantly improved the geopolymerisation process, resulting in enhanced mechanical strength in alkali-activated samples compared to those cured at ambient conditions.

The approach used in the present research reduces the environmental impact by replacing natural with waste material and provides an easy-route for converting various waste into valuable construction resources.



**Figure 1.** The process of pelletization of artificial aggregates from biomass fly ash.

# **Information and Communication Technologies**

# Enhancing Model Interpretability through Variational Bayes: A Single-Tree Alternative to Tree Ensembles

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Ensembles of semi-supervised Oblique Predictive Clustering Trees (SPYCTs) achieve state-of-the-art predictive performance among several structured output prediction (SOP) tasks. However, ensembles limit the interpretability unless using model-agnostic interpretation techniques. Addressing this challenge, we introduce Variational Oblique Predictive Clustering Trees (VSPYCTs) model. Applying the variational Bayes method for determining the oblique splits removes the need for tree ensembles. Through the Bayesian inference, VSPYCTs not only provide predictions but also quantify the uncertainty associated with these predictions, offering profound insights into the model's decision process and confidence levels. As a result we achieve three core objectives. Firstly, it aims to equal or surpass the performance of ensemble SPYCTs through a singular model framework. Secondly, the VSPYCT model is designed to integrate model-specific uncertainty quantification directly into the decision tree framework. Lastly, unlike ensemble methods that combine predictions from multiple trees, VSPYCT retains a streamlined structure for easier interpretation and analysis.

Our extensive evaluation across several benchmark datasets reveals that a single VSPYCT model can either match or outperform a standard ensemble of SPYCTs. Moreover, we present a methodology for extracting feature importance scores and propose an approach for visually interpreting the model's decision-making process, emphasising the significance of features at each decision node, thereby advancing the field of predictive modelling in terms of performance, interpretability, and uncertainty quantification.

# Large Language Models for Efficient Extraction of Relevant Information from Medical Records

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In the healthcare industry, the time-consuming process of manually retrieving information from medical reports significantly reduces the time medical staff can allocate towards patient care. This challenge has prompted the exploration of advanced technologies, particularly generative large language models (LLMs), to understand their efficacy and limitations in simplifying the extraction of relevant data from medical records.

Our study leverages a foundational language model as a starting point and introduces a combination of prompt engineering and fine-tuning techniques aimed at augmenting the model's ability to comprehend this specific task. Prompt engineering is a critical aspect of our approach, involving the development of precise, targeted prompts that direct the model's attention to crucial information within medical reports. This method ensures that the model can distinguish and prioritize the most relevant data, enhancing its efficiency in information extraction tasks. Concurrently, fine-tuning involves adjusting the model's internal parameters to refine its prediction capabilities and text generation in a format that meets specific requirements.

To assess the effectiveness of these enhancements, we employed the F1 score, a harmonic mean of precision and recall, as our primary evaluation metric. The results were promising, showcasing a notable improvement in the model's performance in extracting key information from medical documents compared to the initial foundational language model. Our findings suggest that by incorporating advanced LLM technologies, coupled with strategic prompt engineering and fine-tuning, we can significantly reduce the time spent on manual data retrieval, thereby allowing medical staff to dedicate more resources to direct patient care.

## Acknowledgments:

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## Using equation discovery to analyze ToF-SIMS data in materials science for energy production

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The escalating global energy demand poses a significant contemporary challenge, giving rise to economic crises. Considering the conversion of sustainable energy sources into hydrogen gas as an eco-friendly alternative, we focus on nickel, which historically serves as a primary catalyst for the hydrogen evolution reaction. Several microscopy and spectroscopy techniques have been employed to link the catalytic properties of Ni-based materials to their surface chemistry, including time-of-flight secondary ion mass spectrometry (ToF-SIMS). This analytical tool generates a large amount of data (number of peaks), making it challenging to assign them to specific species on the sample surface.

By employing advanced machine learning methods, we aim to extract information from ToF-SIMS depth profiles to determine species present on the catalyst surface responsible for the electrocatalytic properties of the sample. First, we use hierarchical agglomerative clustering methods to identify species clusters with similar dynamical behaviour, i.e., similar dynamics of change of their intensities. We measure the similarity between a pair of species by using the Spearman correlation coefficient between the corresponding time series. Second, we use the symbolic regression method SINDy to identify arithmetic relations between the species' intensities. The discovered equations optimize the trade-off between the degree-of-fit of the observed intensities and the intensities calculated by the equation, on the one hand, and the complexity of the equation on the other.

## Behaviour Guided Metric for Equation Discovery

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Equation discovery is a machine learning task where we try to find short mathematical equations that fit the given data as best as possible. These equations are more interpretable, efficient to calculate, and usually overfit less than the standard machine learning models. Traditional equation discovery methods rely on syntax-based approaches to generate and evaluate candidate equations, often leading to inefficient exploration of the solution space due to the disconnect between syntactic similarity and actual behaviour. Our work addresses this limitation by introducing a novel stochastic distance metric that measures the similarity between expressions based on their behaviour, not syntax. Results of the experiments with the metric show that it effectively groups together expressions with similar behaviour, leading to a significantly smoother error landscape. This smoother landscape enables better exploration of the space of candidate equations, ultimately leading to the highly efficient discovery of accurate and interpretable equations that describe the underlying phenomena.



## Assessing time-resolved cortico-muscular coupling using dynamical Bayesian inference

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To explore the relationship between cortico-cortical and cortico-peripheral regions, as well as to assess overall brain functioning, connectivity analysis has become increasingly utilized. This study aims to assess cortico-muscular connectivity using wavelet phase coherence and dynamical Bayesian inference methods. The latter is based on the Kuramoto phase model and thus able to detect the effective (directed) connectivity between oscillations.

We concurrently recorded 128-channel electroencephalographic (EEG) and 64-channel high-density electromyographic (EMG) data from twenty participants. Measurements were taken during resting state and while performing an isometric knee extension task, with each leg independently. EMG electrodes were positioned on the Tibialis anterior muscle. Data were down-sampled to 300 Hz, high-pass filtered at 0.5 Hz and low-pass filtered at 150 Hz. We removed 50 Hz line noise using the filtering in power spectrum and, based on manual inspection, removed the segments that contained excessive non-physiological noise. Furthermore, we performed spherical channel interpolation on noisy non-central EEG electrodes, average re-referencing, and independent component analysis to eliminate components that were not of interest.

Subsequent to data pre-processing, time-frequency analysis was conducted using Morlet wavelets. Based on this analysis, time-resolved phase coherence was calculated between activity from each central EEG electrode and the averaged EMG activity from each of the two muscles. Preliminary findings indicate strong beta power (12-30 Hz) and strong gamma power (between 30 – 100 Hz) over central electrodes during motor activity. Moreover, the phase coherence between central EEG electrodes and average EMG electrodes showed high coherence in these frequency bands. Group statistics on the wavelet analysis and dynamical Bayesian inference showed various significant quantities.

The framework of EEG and dynamic Bayesian inference for modelling time-resolved directed connectivity modulations between rest and movement has not been performed previously and with this work we will bring further knowledge with great implications for different neurological diseases.

## A variational autoencoder for n-ary trees

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In science and engineering, many observed systems are modelled using mathematical equations. Knowing these equations is, therefore, crucial for analysing the world we live in. The field of equation discovery is useful for modelling these systems, as it is concerned with discovering algebraic expressions that fit some observed data. One approach to equation discovery is the use of a hierarchical variational autoencoder trained to generate candidate equations [1]. This approach uses binary expression trees to represent expressions and a neural network architecture called a variational autoencoder to generate new expressions. Using binary trees to represent expressions that have functions with less than or more than two arguments requires adding arguments to the function and representing it as a sequence of binary functions, respectively. To avoid this, we upgrade the hierarchical variational autoencoder from [1] with the ability to handle n-ary trees. Apart from functions that do not have exactly two arguments, we also use n-ary tree nodes to represent associative operations, such as addition and multiplication, as operations with an arbitrary number of arguments. We evaluate the effectiveness of our model on such a dataset of n-ary trees by encoding them into a latent space using the encoding part of the autoencoder and reconstructing them with the decoding part. Once we have the reconstructed trees, we evaluate the reconstruction accuracy by calculating the distance between the original and reconstructed expression. Finally, we compare the accuracy of our model to that of the original autoencoder for binary trees. Extending the original autoencoder to include n-ary trees allows it to be used in other fields where the data can be represented with trees, such as abstract syntax trees in computer science or parse trees in computational linguistics.

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# Electric power supply of residential houses by renewable sources assisted by hydrogen storage

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Green technology is becoming increasingly important in reducing carbon emissions from residential houses, for example, through the use of solar panels. However, solar panels alone cannot entirely solve the problem. During the summer months, there is often excess power generated which is put into the grid and it can cause excess of electric energy in the summer period, which cannot be utilized in winter period.

To address this issue, we have developed a long-term energy storage system based on hydrogen technologies. We used real data to create a digital twin, which was then used to simulate and test the system. During the testing phase, we encountered some initial problems in determining the optimal sizes of the components required for the system, including the solar panels, electrolyser, fuel cells, hydrogen storage tank and battery. To optimize the system, we integrated the heat losses of the fuel cell to heat the house, thus reducing electricity consumption of the heat pump. Through different control strategies for energy storage and energy flows, we found a solution for a balancing electric energy generation and consumption over the entire year.

Our promising results have led us to consider improving the system in the future with an automatic optimization algorithm to optimally size system components and minimize the system investment costs. Based on our testing experiences, we have developed different variations of the system which can be applied in residential houses, and we have calculated the estimated cost of the system (Table 1) and resulting price of electric energy.

**Table 1:** Test results of different variations and strategy

Short description of used strategy	Sizes of component					Total investment costs (EUR)	Resulting price of electric energy (EUR/MWh)
	Solar Panel (m <sup>2</sup> )	Electrolyser (kW)	Fuel cell (kW)	Hydrogen tank (kWh)	Battery (kWh)		
<b>a. Operating system</b>	400	0	0	0	130	136 000	688,20
<b>b. With hydrogen system</b>	100	12	8	11 000	16	108 969	469,83
<b>c. Integrated heat</b>	120	8	8	8500	8	84 299	426,58
<b>d. Optimised 1</b>	85	8	6	11 000	10	81 865	414,26
<b>e. Optimised 2</b>	120	4	8	8500	8	79 140	400,47
<b>f. Optimised 3</b>	130	4	4	8500	10	77 312	391,22

## The Challenge of Robot Accuracy – Exploiting Physical Contacts

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Industrial robots excel in repeatability and precision crucial for manufacturing, yet the rise of collaborative robots (cobots) prioritizes safety in human-robot interaction. However, this safety-first approach can undermine precision, notably in tasks with intricate, dynamic motions. Mechanical joint stiffness, inherent in cobots design, can impede desired motion accuracy in such scenarios.

We propose a novel solution to enhance accuracy by leveraging physical contact, inspired by human behavior. Our approach involves intentionally positioning the robot to lean against a stable surface during operation, akin to stabilizing one's hand for fine motor tasks. This external stabilization reduces the impact of joint stiffness and other mechanical inaccuracies, improving precision during dynamic tasks. This concept aligns with human strategies and opens new avenues for cobot design, enabling a balance between safety and precision, crucial in various scenarios.

We have successfully implemented the concept of leveraging physical contact to enhance robotic precision through the implementation of three distinct methodologies, and we are in the process of investigating a fourth. The three implemented methodologies are:

1. Typical inverse kinematics approach, employing primary and secondary tasks.
2. Augmented Jacobian method, combining primary and secondary tasks.
3. Weighted pseudoinverse, utilizing two tasks, with the secondary task weighted with the null space of the primary task. This method is detailed in the article [1].

The main limitation of these methods is solving the inverse kinematics problem, which is not always straightforward, special for big mechanisms. To circumvent the need for inverse kinematics calculation, we now investigate also the applicability of the quadratic programming approach.

Where our objective function aims to minimize robot movement, defined as  $f(q) = \frac{1}{2} q^T q$ , subject to the following conditions:

- The contact force of must remain constant.
- The solution of the forward kinematics problem must be at a minimal distance.
- Minimal movement from the initial position.

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# Nanotechnologies

## Edible lasers

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Edible photonics barcodes and sensors have the potential to revolutionize authentication/tracking systems, especially in the food and pharmaceutical sectors. In the existing markets, the barcodes are predominately printed on product packaging. However, we have developed microlasers in different configurations (such as Whispering-gallery mode (WGM) and Fabry-Perot (FP) lasers) based on completely edible materials for the first time. These microlasers can be placed directly in contact with the food or inside the food packaging to monitor multiple crucial parameters in real time, such as pH, sugar level, and presence of the bacteria. Moreover, this can serve as an edible barcode as well for tracking/authentication against the adulteration or counterfeiting.

## The effect of functionalized gold nanoparticles on cell membrane electroporation

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In recent years, significant progress has been made in the synthesis of metal nanoparticles. Among them gold nanoparticles (AuNPs) have emerged as highly promising due to their distinctive optical and physical characteristics, such as surface plasmon resonance and conductivity. Their high conductivity makes them potentially suitable for enhancement of electroporation [1], [2]. By adding highly conductive gold nanoparticles to cells, theoretically larger induced transmembrane voltage can be obtained consequently enhancing the efficiency of the procedure [3]. Moreover, gold nanoparticles can also act as virtual nanoelectrodes in non-contact electroporation [4].

We synthesized AuNPs of various sizes and shapes to explore their role in electroporation. We synthesized spherical AuNPs with diameter from 10 nm to 130 nm by reducing chloroauric acid with sodium citrate and gold nanorods using the seed-mediated approach. Both types of NPs were functionalized with thiol-terminated polyethylene glycol. Additionally, we synthesized non-conducting silica NPs (by Stöber method) for comparison with conductive gold nanoparticles. For electroporation (Chinese hamster ovary) CHO cells were mixed with nanoparticles (200 µg/ml) and propidium iodide. Changes in cell membrane permeability were detected 3 minutes after electroporation (8x100 µs, 1Hz, Δ E= 0-1 kV/cm). The highest increase in permeability was achieved with AuNP without PEG, while nanorods with PEG and silica NPs had no effect on cell membrane electroporation efficacy. Dynamic light scattering and transmission electron microscopy were used to characterize colloidal stability and morphological aspect of AuNPs, while membrane permeabilization caused by electroporation was assessed using a flow cytometer.

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Acknowledgments: RS ARIS: P2-0089, J2-3043, J2-3046, J3-3079, J7-4420, J2-3040, P2- 0249

## Influence of the functionalisation with catechols on the chemical stability of barium hexaferrite nanoplatelets

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Nanoparticles (NPs) have some exceptional properties due to their nano size and high surface-to-volume ratio. One of these characteristics is high chemical reactivity. It leads to faster and easier dissolution or decomposition of NPs in comparison to coarser particles. To ensure the safe use and disposal of NPs, their possible dissolution and chemical stability should be investigated.

I am investigating the chemical stability of barium hexaferrite (BHF) nanoplatelets (NPLs) synthesized by hydrothermal method. They are one of rare examples of permanent nanomagnets. BHF NPLs can be applied in various technical and biomedical applications including magnetic recording, permanent magnets, magnetic microwave devices and absorbers [1]. We have been investigating the influence of catechol functionalisation on the chemical stability of BHF NPLs. The NPLs were functionalised with catechols (Figure 1) in an aqueous suspension at 80 °C. The surface chemistry properties of BHF were characterized by measuring the zeta potential and their chemical stability was analysed with coupled plasma – optical emission spectroscopy (ICP–OES). The results show that dopamine binds on the surface of BHF NPLs most efficiently. In contrast, the first results suggest that pyrocatechol and caffeic acid induce chemical decomposition of the BHF NPLs.

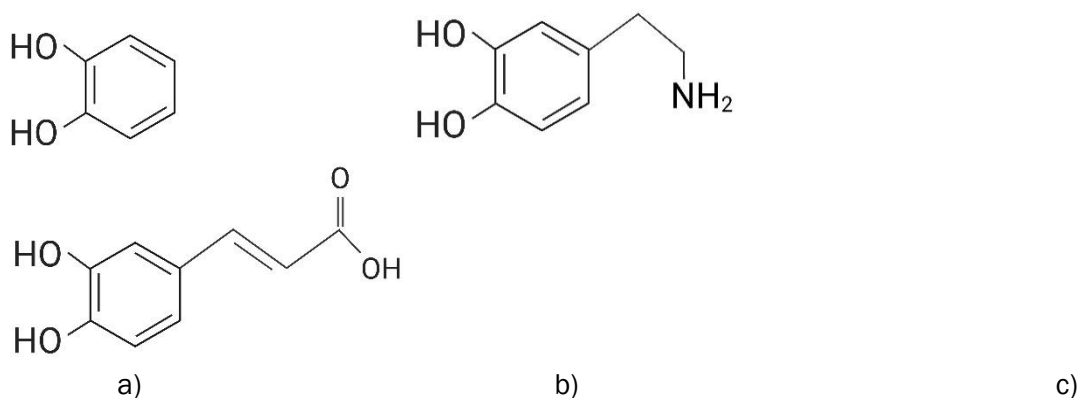


Figure 1: Skeletal formulas of the used catechols, a) pyrocatechol, b) dopamine, c) caffeic acid.

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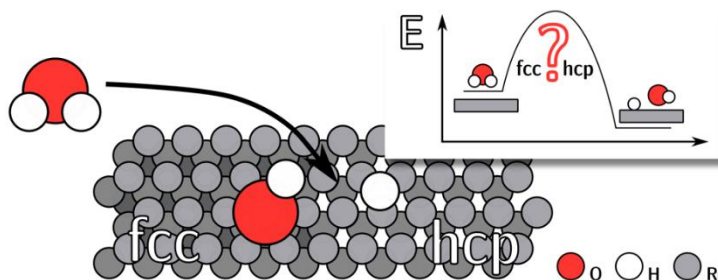
# Structure-Activity Relationship of Ruthenium Catalysts for Hydrogen Evolution Reaction

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**Figure 1.** Comparing the catalytic activity of fcc- and hcp-Ru towards hydrogen evolution reaction.

The hydrogen evolution reaction (HER) is a half-reaction of water electrolysis, an environmentally friendly way to produce hydrogen gas. Commercial catalysts for HER typically contain platinum, a metal that is both expensive and scarce. One interesting alternative material is ruthenium, known for its high activity in alkaline conditions. Ruthenium crystallizes in the hexagonal close-packed (hcp) structure. However, for some supported Ru nanoparticles, the face-centered cubic (fcc) structure was observed, and it showed high HER activity [1]. This observation begs the question of whether the high activity of fcc-Ru nanoparticles is due to the fcc structure itself or strong metal-support interaction. To our knowledge, only one study addresses the role of Ru structure towards HER with density-functional theory (DFT) [1], which reports surprisingly high differences in adsorption and activation energies between fcc- and hcp-Ru. In particular, fcc-Ru adsorbs hydrogen significantly weaker and displays lower activation energy for water dissociation than hcp-Ru, making fcc-Ru more active for alkaline HER. To verify these claims, we performed DFT calculations of hydrogen adsorption and water dissociation on hcp- and fcc-Ru. Our results reveal little difference in hydrogen adsorption energy between hcp- and fcc-Ru. In the analysis of the water dissociation reaction, none of the used water models predicted substantial differences in activation barriers between hcp- and fcc-Ru. Our findings suggest that the observed high activity of supported fcc-Ru nanoparticles cannot be attributed solely to their fcc structure, suggesting an important role of strong metal-support interaction. Further research with realistic models of supported nanoparticles is necessary to verify this suggestion and better explain the high activity of supported Ru nanoparticles.

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Acknowledgments:

The authors would like to thank the Laboratory for Eletrocatalysis at the National Institute of Chemistry for motivating the study of HER on Ru catalysts.

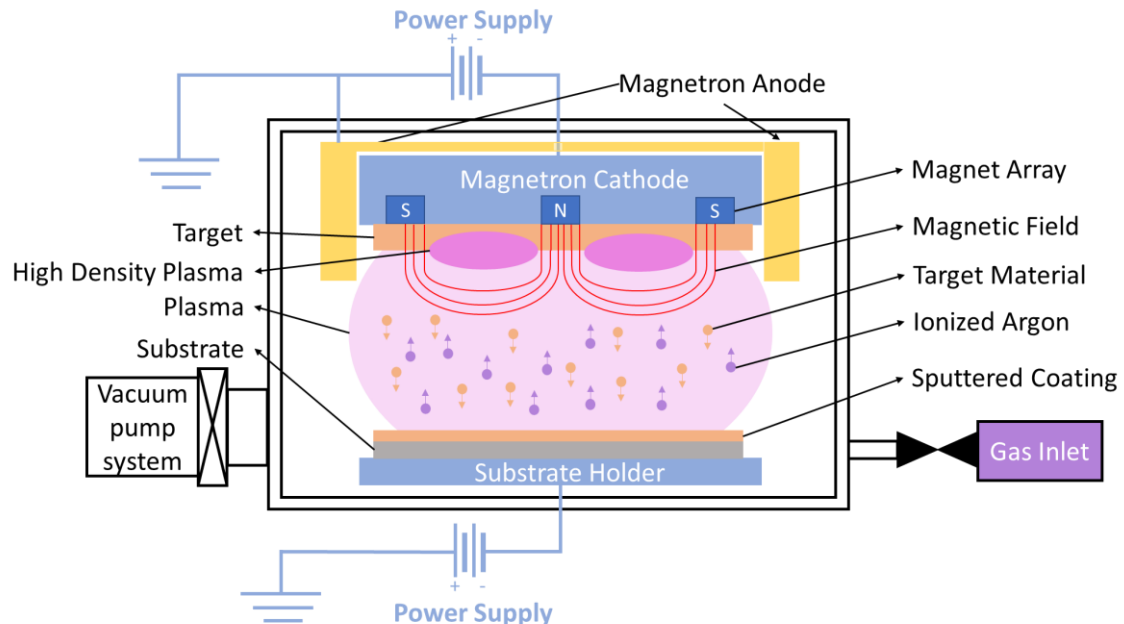
## Using a novel approach to design a versatile lab-scale magnetron-sputtering deposition system

Žan Gostenčnik<sup>1,2\*</sup>, Aljaž Drnovšek<sup>1</sup>, Matjaž Panjan<sup>1</sup>, Matej Drobnič<sup>1</sup>, Miha Čekada<sup>1,2</sup>

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**Figure 2:** Schematic representation of the magnetron sputtering deposition system

Magnetron sputtering (Figure 1) is one of the most used physical vapor deposition (PVD) techniques for the deposition of thin films. Creating optimal sputtering conditions involves introducing an inert gas, typically argon, into the vacuum chamber once the desired pressure is achieved. When an electric field is applied between the electrodes of a magnetron, argon is ionized to form a plasma. Positioned in front of the cathode, the target is bombarded by positively charged ions from the ionized gas, causing it to eject the target particles. These particles then deposit onto the substrate surface, facilitating thin film growth. Enhancing inert gas ionization is achieved by the application of a magnetic field with the use of a magnet located behind the cathode in the magnetron [1].

Our work intended to build a versatile thin film deposition system. We used the vacuum chamber of an old industrial deposition system with an attached system of two pumps- a rotary vane pump and a turbomolecular pump. We mounted the magnetrons and substrate holder inside the chamber and connected them with a direct-current power supply. We added a heating system and gas inlets-argon for plasma and nitrogen for reactive depositions. With this deposition system, we can tailor the growth of alloy and ceramic thin films by adjusting deposition parameters such as magnetron power, temperature, pressure, and bias.

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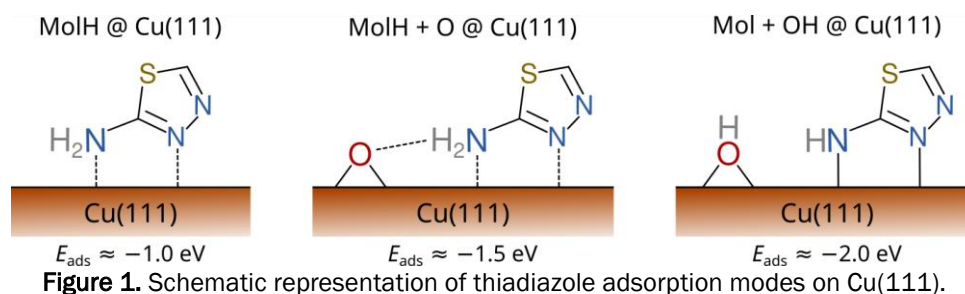
## Adsorption of thiadiazoles on Cu(111) promoted by chemisorbed O: a DFT study

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The study of adsorption modes of organic molecules on metal surfaces is crucial for understanding corrosion inhibition mechanisms. We explored the adsorption behavior of six thiadiazoles on copper with density-functional theory (DFT) calculations, focusing on how chemisorbed oxygen affects their adsorption energies. Thiadiazoles adsorb moderately on bare Cu(111) with adsorption energies of about  $-1$  eV. However, their adsorption becomes considerably stronger in the presence of chemisorbed O atoms. Stronger adsorption is the consequence of a few effects. The first is the indirect O-induced strengthening of the molecule–surface bonds by about 0.2 eV. Molecules capable of forming hydrogen bonds could further stabilize by H-bonding with the chemisorbed O atoms, resulting in an additional stabilization of approximately 0.3 eV. Consequently, chemisorbed oxygen leads to an overall stabilization of adsorbed intact thiadiazoles by approximately 0.5 eV, resulting in adsorption energies of about  $-1.5$  eV. Adsorbed thiadiazoles can further stabilize by 0.5 eV by the O-induced cleavage of their X–H bond (X = N or S) via the  $\text{MolH}_{(\text{ads})} + \text{O}_{(\text{ads})} \rightleftharpoons \text{Mol}_{(\text{ads})} + \text{OH}_{(\text{ads})}$  reaction, where the labels MolH and Mol designate an intact and deprotonated thiadiazole molecule, respectively. As a result, their final adsorption energies are about  $-2$  eV, indicating strong adsorption of thiadiazoles on copper surfaces. These findings align with our team's prior observations, highlighting the significant role of chemisorbed oxygen in enhancing the adsorption of azoles on copper [1, 2].

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## Systematic investigation of the copper (I) chloride – HCl - triethylenediamine system in composition space diagram

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In the present study, the copper (I) chloride – HCl - voluminous organic polyamine composition diagrams were discovered. Earlier published articles, which describe the synthesis and characterization of organic polyamines chlorocuprates, do not cover all possible coordination compounds potentially present in these systems. This was the reason for the systematic investigation of these systems based on the use of two-dimensional composition diagrams.

Electrochemical syntheses were carried out using copper wire electrodes, CuCl<sub>2</sub>, HCl, and triethylenediamine (1,4-diazabicyclo[2.2.2]octane or DABCO) as starting reagents and ethanol as solvent. The obtained compounds were characterized by single-crystal X-ray diffraction and Raman spectroscopy.

In some areas of the composition diagrams, the formation of already-known compounds was observed [1-4]. Otherwise, two new coordination compounds were obtained. The compound [C<sub>6</sub>H<sub>13</sub>N<sub>2</sub>]<sup>+</sup>[Cu<sub>2</sub>Cl<sub>3</sub>]<sup>-</sup> contains a monoprotonated Hdabco<sup>+</sup> cation coordinated to the Cu<sup>I</sup> ion *via* an unprotonated N1 (Fig. 1). Both crystallographically independent copper centers are three-coordinated. Due to the bridging function of the Cl atom infinite cuprochloride chains running along the b-axis appear.

The crystal structure of the compound Cu<sub>2</sub>Cl<sub>2</sub>C<sub>6</sub>H<sub>12</sub>N<sub>2</sub> contains a neutral DABCO ligand coordinated to copper centers. Each metal ion is coordinated by a nitrogen atom of DABCO and 2 bridging chlorine ions. The inorganic part of the structure is represented as infinite (CuCl)<sub>n</sub> chains.

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## Unraveling anisotropic behavior of $\text{LiNi}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2$ through controlled epitaxial thin film growth via pulsed laser deposition

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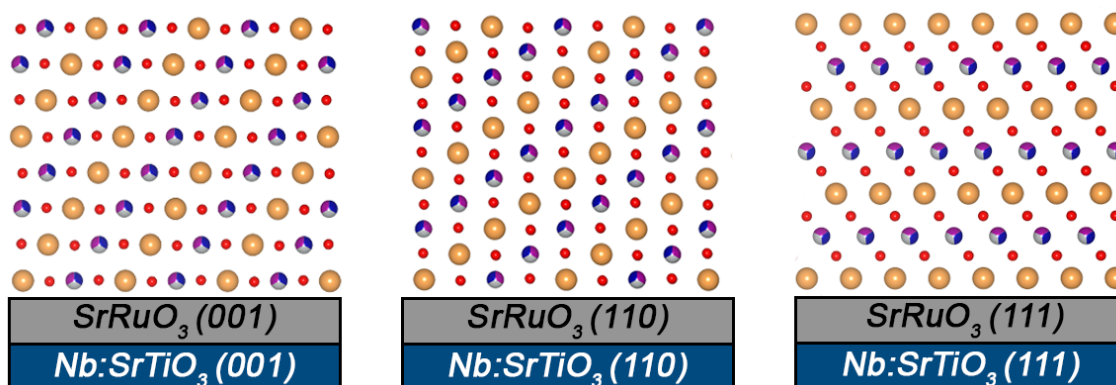
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$\text{LiNi}_{1-x-y}\text{Mn}_x\text{Co}_y\text{O}_2$  (NMC) is a promising class of cathode materials for lithium-ion batteries [1]. Since NMC exhibits a two-dimensional layered crystal structure, with alternating slabs of lithium and transition metal cations, the ionic transport of lithium from the bulk to the surface is strongly dependent on the crystal orientation. Pulsed laser deposition (PLD) is a powerful technique for the preparation of ceramic materials in the form of epitaxial thin films, which proved to be valuable for exploring the anisotropic properties of layered materials [2].

PLD was used for thin film deposition of NMC on  $\text{SrRuO}_3/0,5\% \text{wt Nb-doped SrTiO}_3$  (SRO/Nb:STO) substrates with different crystal orientations. Epitaxial growth of NMC thin films was proved by X-ray diffraction, resulting in (104), (118) and (003) out-of-plane oriented NMC, deposited on (001), (110) and (111) substrates, respectively. Microstructural analysis revealed the presence of twinned domains in NMC thin films grown on (001) and (110) SRO/Nb:STO, due to the tilted growth of the layered structure, but no twinning was observed in the film, grown on (111) SRO/Nb:STO. Furthermore, differently oriented NMC thin films were electrochemically characterized in the half-cell configuration. Galvanostatic cycling at different rates showed that the crystal orientation of NMC plays a significant role in the electrochemical performance of the NMC at higher charge/discharge rates, proving the anisotropic behavior of lithium transport in NMC.



**Figure 1.** Different orientations of lithium layers in epitaxial NMC thin films, deposited on SRO/Nb:STO (001), (110) and (111) out-of-plane oriented substrates.

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## Low-cost catalysts for green hydrogen generation through water splitting

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The net zero emission strategies of energy conversion and storage are crucial for the future. Hydrogen can be used as a clean and sustainable energy vector that can be integrated with the renewable sources to fulfil clean energy demands. Water electrolysis is one of the cleanest ways to produce green hydrogen. From the current electrolyzer technologies, anion exchange membrane water electrolyzer (AEMWE) stands apart due to its cost effectiveness and the use of non-noble metal catalysts. The development of more affordable, high-performing catalysts will further increase the efficiency of the AEMWEs, leading to a reduction in hydrogen production costs. Amongst the low-cost electrocatalysts, metal borides have turned out to be one of the most ideal ones for incorporation in AEMWEs. Our research is focused on discovering multi metallic borides than can attain higher activity than the already reported mono metallic borides. Our work emphasises on the combinations of transition metal borides including low-cost metals such as Co, Fe, Ni, Mo and W. The best catalysts will also be investigated in saline water conditions to explore their potential for direct seawater electrolysis.

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## Copper patina as a form of corrosion protection

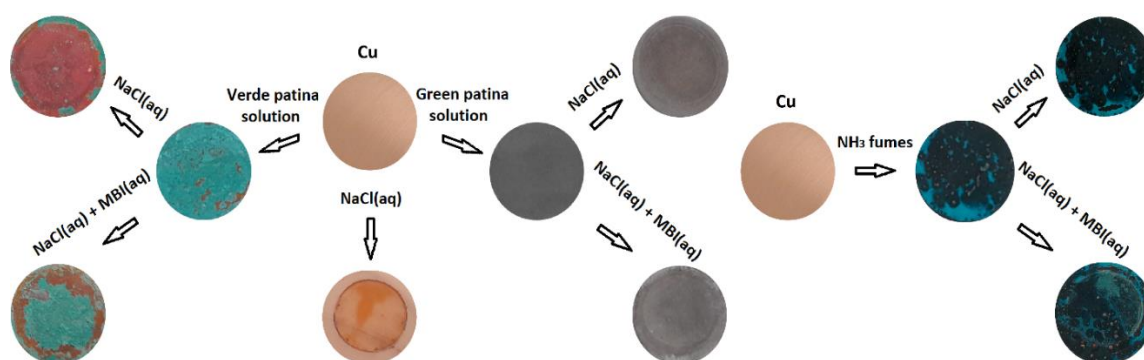
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Corrosion is a spontaneous process of metal degradation when a metal surface is exposed to the environment, resulting in the surface being covered in oxides, phosphates or sulfides, which exhibit mechanical properties similar to ore. In some cases, corrosion products on the metal surface are stable and can suppress or completely stop the progression of the corrosion process. One such product is patina. This study investigated patina formation on copper and its effect on corrosion progression. First, copper samples were prepared by wet grinding and chemically treated. Three types of patina were then prepared by using prescribed procedures for Green and Verde patina solutions, while the third patina was produced by Ammonia fumes. Patinated copper samples were then electrochemically tested in 0.1 M NaCl solution.

The study showed a direct correlation between the roughness of the surface patina and its ability to protect the underlying metal. In the case of the Verde patina, the top layer of the surface was rough and easily damaged, so the corrosion freely advanced, while in the case of the Green patina, the surface was smooth and highly resistant to mechanical damage. Green patina proved highly effective against corrosion damage. Furthermore, it was discovered that while patina creates a protective layer, it does not negate the effect of corrosion inhibitor 2-mercaptobenzimidazole added to NaCl solution, but rather its presence additionally improves corrosion resistance [1].



**Figure 1:** Schematic presentation of copper surface changes during the experiments.

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## The influence of process conditions on ZnO nanorods formation and their photocatalytic caffeine degradation efficiency

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Organic pollutants such as caffeine significantly burden the environment [1-3]. These substances are released in large quantities, polluting water sources, soil, and air [1-3]. In recent years, much research has been invested in developing effective methods to remove these pollutants [2, 3]. Zinc oxide (ZnO) shows potential as a catalyst in the degradation of organic pollutants through photocatalysis [3]. However, improving and optimizing its photocatalytic efficiency proved to be a tedious task.

Our study affirms the potential of ZnO nanorod arrays in water purification and caffeine removal; however, such a similar product also exhibits a wide efficiency gap. In this research, we synthesized ZnO nanorod arrays using a two-step process. Initially, a ZnO seed layer was deposited onto a glass substrate, followed by hydrothermal growth at different growth times to form nanorod-like arrays; the films were subsequently subjected to different annealing temperatures. Material parameters were analyzed by scanning electron microscopy (SEM), X-ray and optical spectroscopies, and thermogravimetry (TG) analysis. The photocatalytic activity was assessed via UV-Vis spectrophotometry during caffeine degradation. The results indicate that additional annealing has virtually no effect on the morphology and structure of the nanorods. Nonetheless, it has a significant impact on ZnO's photocatalytic efficiency. Such results are important to finding a suitable environment for ZnO production, especially during such inexpensive temperature processes, and are vital for understanding the physical processes involved during photocatalytic degradation.

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### Acknowledgments:

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## Corrosion protection of AZ31 magnesium alloy using sol-gel coating

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Magnesium (Mg) alloy stands out as one of the lightest structural materials, and it finds application in different industries such as aerospace, automotive, and biomedicine. But Mg alloy such as AZ31 (composed primarily of magnesium ~96%, along with small amounts of aluminium ~3%) and zinc ~1%) has low corrosion resistance in environments containing chloride ions, a. g. NaCl solution [1]. Several environmentally friendly surface treatments have been studied because the surface preparation affects the magnesium alloy resistance [1]. In addition, coating deposition can enhance resistance; one promising technique is hybrid sol-gel coating.[2]

This study aims to investigate the effect of surface preparation methods on the corrosion resistance and deposition of hybrid sol-gel coating AZ31 alloy. Surface characterization of AZ31 after three surface preparations (grinding, polishing, and heat treatment) was conducted using scanning electron microscopy coupled with an energy-dispersive spectroscope and contact profilometer for assessing composition and surface topography. The coating was prepared from organic precursors 3-(methacryloyloxy)propyl trimethoxysilane (MAPTMS) and methyl methacrylate (MMA) and inorganic precursor tetraethyl orthosilicate (TEOS) [2]. Corrosion properties of hybrid sol-gel coating applied on AZ31 alloy were evaluated by electrochemical impedance spectroscopy measuring during immersion in 0.1 M NaCl.

The results confirmed that surface preparation methods affect the corrosion resistance of AZ31 alloy and the formation of the deposited hybrid sol-gel coating. The electrochemical results reflected a few months of durable corrosion protection; therefore, this type of coating presents very promising corrosion protection for future studies.

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## Assessing Feasibility of Corrosion Resistance Evaluation Techniques for Zirconium Conversion Coatings on Zinc

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Conversion coatings, where, as the name implies, the surface of a metal is converted into one with better properties, mainly serve as primers for enhancing corrosion resistance and paint adhesion in the aircraft and automotive industry. Among the eco-friendly options, zirconium conversion coatings (ZrCC) have emerged as promising candidates [1]. However, the literature still lacks a consensus on the optimal conditions and evaluation techniques for these coatings.

To bridge this gap, we employed statistics in the form of Response Surface Methodology (RSM) to assess the individual and mutual effects of a wide range of Zr conversion bath parameters (concentration of  $\text{H}_2\text{ZrF}_6$ , pH and conversion time) on corrosion resistance of zinc. Corrosion resistance responses were measured using different techniques, namely, protective ability (PA) from a so-called drop test, polarization resistance ( $R_p$ ) from potentiodynamic polarization curves (PPC), and the value of absolute impedance ( $|Z|$  at 0.25119 Hz) from electrochemical impedance spectroscopy (EIS).

While RSM models for PA and  $|Z|$  at 0.25119 Hz proved effective in identifying optimal conditions, it was found that the model for  $R_p$  was insignificant, rendering it impractical for evaluation. This inadequacy was further revealed through the analysis of EIS spectra and Scanning Electron Microscopy/Energy Dispersive X-ray Spectrometry (SEM/EDS), indicating the diffusion-controlled nature of Zn corrosion associated with ZrCC at  $\text{pH} > 4$ . This lays the groundwork for future research on various substrates and additives.

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### Acknowledgements:

The assistance from Prof. dr. Davorin Kramar (University of Ljubljana, Faculty of Mechanical Engineering) in analyzing the RSM data is greatly appreciated.

## Hydrogen Separation with Membranes: Accounting for the Interference Effect in Quadrupole Mass Spectrometers

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Hydrogen, the clean carrier, is expected to play an important role in our journey towards green energy. Yet, in conventional hydrogen production lines, efficient separation measures are required due to the simultaneous release of other gases [1]. While noble metal membranes provide high hydrogen selectivity, their reliance on limited resources and proneness to embrittlement necessitate the search for alternative approaches. Two-dimensional nanomaterials offer a promising alternative for low-temperature separation [2], [3]. Accurate evaluation of the effectiveness of such nanostructured membranes in separating hydrogen from mixtures requires information on all permeating species. Quadrupole mass spectrometers (QMS) aid in identifying and quantifying the permeated species, but challenges arise from the instrument's sensitivity dependence on the composition of the mixture [4]. This phenomenon is known as the interference effect, and our research aims to explain how it impacts hydrogen quantification with QMS. We established a calibration method useful in dynamic operational settings, where gas flow rates vary with time. This broad range calibration approach offers practical benefits over standard single-point methods, improving hydrogen quantification accuracy up to a factor of 2.5. It provides means of careful evaluation, enabling opportunities for advancements in membrane technologies for hydrogen separation.

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### Acknowledgements:

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## Crystallographic defects in cold-sintered ferroelectric ceramics

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Perovskite oxides of general formula  $ABO_3$  are multifunctional materials that accommodate elements of different size and charge on their A and/or B sites, as well as point defects, e.g., vacancies, and other crystallographic defects by strain and charge redistribution. This versatility results in compounds exhibiting a variety of functional responses and their coupling, from e.g., mechanical, electrical, caloric, to photovoltaic and piezo-catalytic effects [1]. Besides finding new materials with novel functionalities, their development aims at designing materials from non-toxic elements, but also processing technologies that are energy-efficient and cost-effective. Such an innovative technology is the cold-sintering process (CSP) that deviates from conventional sintering methods by using a transient liquid phase and high pressures (up to 600 MPa), and a significantly decreased sintering temperature (300 °C or less), to densify the material and enable control of the microstructure [2].

During the CSP of ferroelectrics such as  $BiFeO_3$  (BFO) and  $K_{0.5}Na_{0.5}NbO_3$  (KNN), that are characterized by a switchable polarization under an external electric field, crystallographic defects (dislocations) are induced in the material, which are associated to strain due to the applied pressure. These can significantly influence the movement of domain-walls (separating adjacent ferroelectric domains of homogeneous polarization) and change the materials properties [3]. Scanning Transmission Electron Microscopy (STEM) is the optimal tool to analyze dislocation landscape, unraveling their formation, propagation through careful examination and quantitative analysis of lattice distortions, and their interaction with the domain walls. Image processing techniques, such as geometric phase analysis (GPA), can provide valuable insights into dislocation behaviour and strain conditions in ceramics. Such an analysis of lattice distortions and defect states in selected cold-sintered ferroelectrics will be presented in this contribution. We aim to explore how cold-sintering affects defect structures in perovskite ferroelectrics, providing insights for sustainable and high-performance ceramics.

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## Investigating Lithium metal dendrite growth by Magnetic resonance imaging

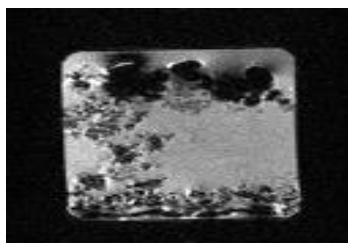
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Lithium metal batteries with higher energy densities can be used as a forefront battery technology once the challenges related to safety are overcome. The needle-like dendrites that grow on the anode during lithium plating and stripping which result in capacity fading put forward a major safety concern [1]. It might reach the cathode during charging and can lead to battery shorting. In order to find ways that can mitigate this dendrite growth, it is essential to learn more about its process of formation. Magnetic resonance imaging is a unique technique that can be used for in situ imaging of the process taking place inside a working cell and can thus give valuable insights into these microstructure growths [2]. To begin with, we designed a suitable model of a symmetric Lithium metal cell that can be imaged and studied using MRI. The cell consists of two lithium metal electrodes, LiPF<sub>6</sub> in EC/DMC electrolyte, and Copper current collectors. The dendrite growth was studied by applying current in both positive and negative directions. Application of current in the positive direction resulted in a uniform dendrite formation from one of the electrodes, once the current was reversed an uneven distribution of dendrites along with the formation of some gas bubbles from the other electrode was observed (Figure 1). Thus, investigating the scope of MRI and the effect of current densities and cell geometries in lithium dendrite growth will give a future direction to optimise and design safer lithium batteries.



**Figure 1.** MRI Slice of dendritic growth in a battery cell.

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## Evaluation of hydrostatic properties of selected halogenated fluids under high pressure

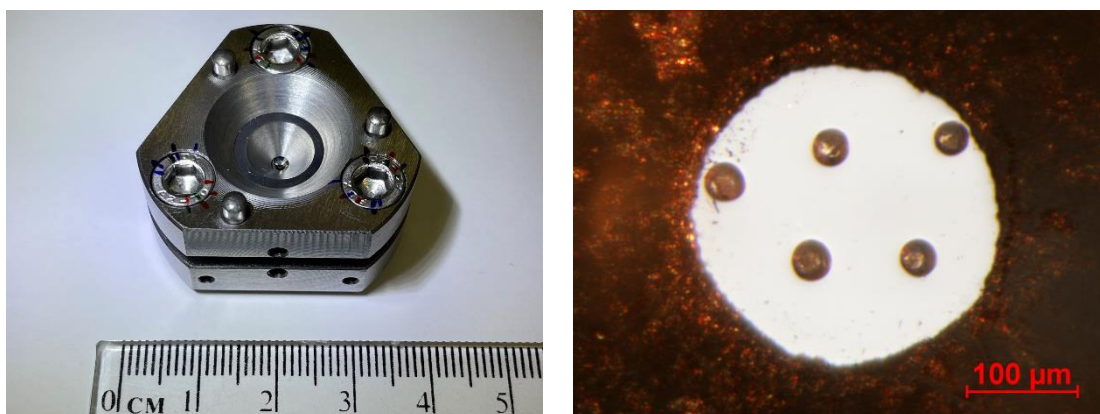
**Klemen Motaln<sup>1,2\*</sup>, Erik Uran<sup>1,2</sup>, Matic Lozinšek<sup>1,2</sup>**

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Diamond anvil cell (DAC) is a powerful and convenient tool for achieving pressures in the gigapascal (GPa) range and allows for materials to be studied *in situ* using a variety of characterisation techniques. A key component of the DAC experiment is the pressure transmitting medium (PTM), which ensures that the pressure is uniformly distributed throughout the sample chamber. The PTM should remain hydrostatic over the entire studied pressure range, as non-hydrostatic conditions can have a detrimental effect on the sample crystallinity and even lead to amorphisation [1]. Commonly used PTMs include inert gases (e.g., N<sub>2</sub>, He, Ne), which are hydrostatic to more than 10 GPa and require special instrumentation for loading [2]. Alternatively, methanol–ethanol, *n*-pentane–isopentane mixtures and silicone oils are easier to handle and have a comparably high hydrostatic range [2] but may react with the materials under investigation. The use of halogenated fluids as PTM provides a chemical resistivity comparable to that of the inert gases, but it has been shown that all such fluids investigated to date have a hydrostatic limit below 2.5 GPa [2, 3]. In this work, the hydrostatic performance of the halogenated fluids Fomblin Z25, Fomblin Z60, Fomblin Y-LVAC 06/6, and Halocarbon oil under high pressure was investigated for the first time. The selected fluids were placed in Merrill-Bassett type DACs, using Inconel X750 as the gasket material and loaded with ruby spheres evenly distributed throughout the sample chamber (Figure 1). The pressure at different positions in the cell was deduced from the position of the *R*<sub>1</sub> ruby fluorescence line [4], and the hydrostaticity of the medium was inferred from the observed pressure gradients.



**Figure 1.** Merrill-Bassett type DAC (left) and sample chamber of a DAC loaded with ruby spheres and a PTM (right).

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## Manufacturing of complex ceramic parts by light patterning of photoactive resin

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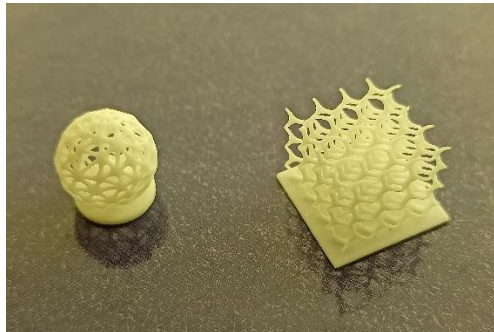
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Production of complex ceramic parts by classical processing methods is highly challenging and costly due to the need for complex moulds and rapid tool wear [1]. In recent years, additive manufacturing technology has become an increasingly attractive family of techniques for rapid prototyping and manufacturing of complex parts made of various materials. One such technique is stereolithography (SLA), in which a liquid resin of photoactive precursors is polymerized into a solid object by the application of patterned light in a layer-by-layer fashion. By addition of ceramic powders into such resins and subsequent postprocessing of the printed part, a dense ceramic object of complex shape can be produced. Two such objects are presented in Figure 1.

Future research in this topic will focus on tailoring the photoactive blends for diverse applications that require complex shaping of technical ceramics. The main goal is the adaption of resin mixtures to electro-ceramic powders for on-demand modular production of complex electrical components. Additionally, testing of ceramic composite materials for high-performance structures for impact protection will be carried out. Finally, new photo-binding mechanism will be researched.



**Figure 1.** Dense alumina objects prepared by the SLA technique.

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## Thrust force generated by surface dielectric barrier discharge

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Surface dielectric barrier discharge (SDBD) creates cold atmospheric plasma by applying a high-voltage electrical field between electrodes separated by a dielectric. This ionization process, in which charged particles collide with neutral ones, induces a thrust force. This study investigates the effects of dielectric thickness and electrode spacing on thrust force, focusing on voltage frequencies of 1 kHz and particularly above 20 kHz, where the behavior of thrust force at such high frequencies remains largely unexplored. For our force measurements, we utilized an analytical balance with a precision of 1 mg. We experimentally analyzed the influence of discharge geometry and related phenomena on thrust force and its behavior over time. We discovered that utilizing a thinner dielectric increases thrust at the given voltage, and reducing the diameter of the wire used for the exposed electrode also enhances the thrust. However, if the width of the insulated electrode is insufficient, the force will plateau at a certain voltage and cease to increase. This limitation is not observed when the insulated electrode is sufficiently wide. Optimal thrust was achieved with electrodes offset by approximately 1 mm, regardless of voltage or electrode width. The direction of the force was measured at around 10° relative to the dielectric surface, irrespective of voltage amplitude, electrode width, or voltage frequency. Time-based analysis revealed that the force weakens over time, which becomes particularly noticeable at higher power settings. Using IR temperature analysis, we showed that the force decline correlates with air heating above the dielectric, confirmed by oscilloscope discharge measurements. These findings contribute to understanding airflow regulation in various applications.

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## Structural insights into Vaa-snaclec-3/2 antiplatelet activity

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Animal venoms contain diverse and highly specific pharmacologically active substances that make them a rich source of novel drug candidates. The venom of Europe's most venomous snake, the nose-horned viper (*Vipera a. ammodytes*), contains mainly protein toxins that affect the haemostatic system. Among other effects, it induces a severe but transient and reversible thrombocytopenia without bleeding [1]. By *in vitro* and *in vivo* experiments, we confirmed Vaa-snaclec-3/2 as the toxin responsible for this effect. This protein is a member of the functionally diverse family of C-type lectin-like snake venom proteins (snaclecs). While snaclecs typically form heterodimers of alpha and beta subunits, they can also associate into diverse homo-oligomers. Vaa-snaclec-3/2 has been shown to bind to the glycoprotein Ib receptor (GPIb) on the platelet surface, joining in this way two to three platelets into small agglutinates without causing their activation. In view of its potential medical application as an alternative agent to prevent the formation of blood clots during surgical interventions in angiology and cardiology, we decided to investigate its mechanism of action in more detail. In particular, we have been analysing the relationship between the primary structure of Vaa-snaclec-3/2, its oligomerization state and activity. To this end, we are using multiple sequence alignment, tertiary structure analysis tools and mass spectrometry. The ultimate goals of our project are to improve our understanding of the mechanism of action of Vaa-snaclec-3/2 and to be able to predict physiological activity of other snaclecs that still has to be characterized.

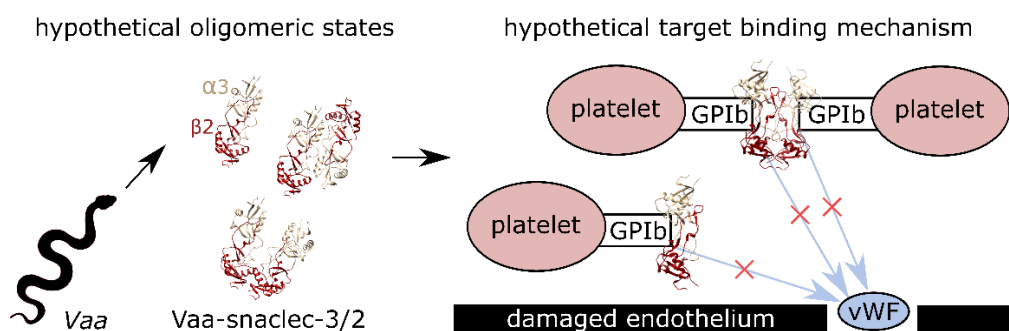


Figure 1. Graphical abstract.

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### Acknowledgments:

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## Optimizing Recycled Nd-Fe-B Magnets via Single Grain Boundary Engineering

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Nd<sub>2</sub>Fe<sub>14</sub>B permanent magnets were discovered in 1984 [1] and are now crucial components in many fields of technology. In recent years, the research on Nd-Fe-B permanent magnets has moved from achieving better performance to balancing performance and environmental sustainability. Efforts in this direction entail simultaneously optimizing coercivity and remanence, decreasing reliance on heavy rare earth, and incorporating recycled materials [2].

Hydrogen Processing of Magnetic Scrap (HPMS) is one recycling method for end-of-life (EOL) magnets [3]. However, high oxygen levels and other impurities often reduce the magnetic performance of HPMS-based powders. In our research, recycling includes the elimination of existing secondary phases from recycled HPMS material to obtain single-phase Nd<sub>2</sub>Fe<sub>14</sub>B material. Following this, a bottom-up approach is implemented to redesign the microstructure of the recycled magnets and enhance their magnetic performance. A fresh non-magnetic material (Nd<sub>70</sub>Cu<sub>30</sub> low eutectic alloy) was introduced in various amounts (0 to 30 wt%). The mixture was then consolidated via Spark Plasma Sintering (SPS).

The incorporation of Nd-Cu alloy into the system has demonstrated several advantages. Full density (7.6 g/cm<sup>3</sup>) was reached with a 10 wt.% Nd-Cu addition and the remanence was also saturated at 1.04 T. Increasing the Nd-Cu addition beyond 10 wt% was demonstrated to reduce the volume fractions of the Nd<sub>2</sub>Fe<sub>14</sub>B hard-magnetic phase. However, the remanence remains stable due to improved grain crystallographic alignment. Coercivity increases from 50 to 826 kA/m as the Nd-Cu addition rises from 2.5 to 30 wt%, attributed to oxygen redistribution and Nd<sub>2</sub>O<sub>3</sub> formation within triple pockets. This facilitates the formation of a grain boundary phase and enhances grain wettability.

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### Acknowledgments:

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## A novel compound with Xe–N bond: [NCCH<sub>2</sub>CN–XeF][AsF<sub>6</sub>]-HF

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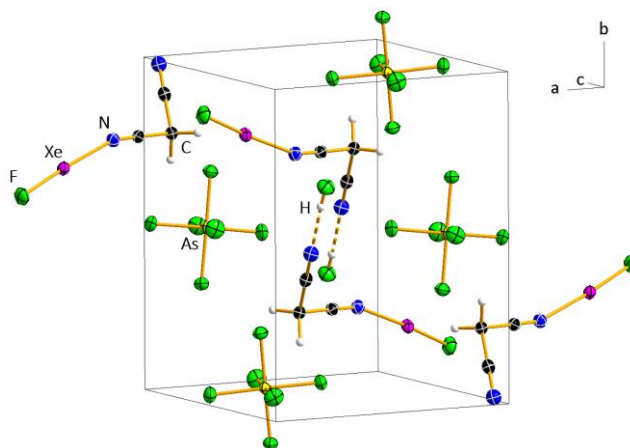
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The [RN–Xe–F]<sup>+</sup> adduct cation species represent one of the largest family of compounds where noble-gas element is bonded to nitrogen. Nevertheless, the choice of nitrogen-donor Lewis base is limited to a small selection of nitriles RCN (R = H, CH<sub>3</sub>, CH<sub>2</sub>F, C<sub>2</sub>H<sub>5</sub>, (CH<sub>3</sub>)<sub>3</sub>C, C<sub>2</sub>F<sub>5</sub>, C<sub>3</sub>F<sub>7</sub>, C<sub>6</sub>F<sub>5</sub>) and a handful of fluorinated molecules (C<sub>5</sub>F<sub>5</sub>N, 4-CF<sub>3</sub>C<sub>5</sub>F<sub>4</sub>N, s-C<sub>3</sub>F<sub>3</sub>N<sub>3</sub>), which are resistant to oxidation and fluorination by highly reactive XeF<sup>+</sup> salts [1–4]. In this type of compounds, an Xe–N interaction takes place between the lone electron pair of the nitrile and the Lewis acid XeF<sup>+</sup> [1]. To explore and expand the limited chemistry of Xe<sup>II</sup>–N-bonded compounds, we investigate polytopic nitrogen bases.

In this work, a ditopic donor malononitrile, NCCH<sub>2</sub>CN, was reacted with the Lewis acid [XeF]<sup>+</sup>[AsF<sub>6</sub>]<sup>–</sup> in anhydrous HF at low temperature. The novel compound [N≡C–CH<sub>2</sub>–C≡N–Xe–F]<sup>+</sup>[AsF<sub>6</sub>]<sup>–</sup>-HF, which is stable only at low temperatures was isolated and structurally characterised by the low-temperature single-crystal X-ray diffraction and by low-temperature Raman spectroscopy. In the resulting adduct cation XeF<sup>+</sup> is bonded to only one –CN group, whereas the second one is hydrogen-bonded to HF (Figure 1). These findings expand the limited class of structurally characterised Xe–N-bonded adduct cations.



**Figure 1.** The crystal structure of [NCCH<sub>2</sub>CN–XeF][AsF<sub>6</sub>]-HF. Thermal ellipsoids are shown at the 50% probability level.

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## In-situ Electrochemical Liquid Cell TEM study of copper electrodeposition and electro-dissolution during potential cycling

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Electrodeposition is a vital technique for a myriad of processes, ranging from the coating of electrodes[1] to the synthesis of electro-active nanoparticles[2], to name a few applications. The efficiency of this technique is directly correlated with the ability to control the material's final morphology and structure and, therefore, its final properties. In particular, the initial stages of nucleation and growth comprise a series of yet-to-be-understood processes that play an integral part in the final properties of nanoparticles. These processes can be assessed through *in-situ* Liquid Cell Transmission Electron Microscopy (LCTEM), which is an advanced experimental microscopy technique that allows one to probe nanoscale structural and chemical dynamic changes of a system in a liquid environment as close as possible to its native conditions. Consequently, we employed a correlative methodology for *in-situ* electrochemical LC-TEM experiments to study the dynamics of Cyclic Voltammetry (CV) in electrodeposition and electro-dissolution of copper nanoparticles.

The *in-situ* LCTEM experiments were studied using a JEOL JEM 2100 TEM (JEOL, Japan) at 200 kV accelerating voltage—the liquid TEM holder Protochips Poseidon (Protochips, USA). The electrolyte used was 1 mM CuSO<sub>4</sub> + 10 mM H<sub>2</sub>SO<sub>4</sub>. Cyclic voltammetry (CV) was the electrochemical technique chosen to study the dynamic behavior of copper electrodeposition within a potential window of -1 V to +0.5 V vs. Pt pseudoreference electrode.

The cyclic voltammetry was used for characterizing an electrochemical system. Oxidation and reduction peaks were measured at -0.4 V vs. Pt and -0.8 V vs. Pt, respectively. At the reduction inset potential, the nucleation of islands was simultaneously recorded. As potential swept more negatively, these particles turned into dendrites. As for the oxidative part of the experiment, profound dynamic morphological changes always anteceded the dissolution of the nanoparticles. Probing the dynamic of Cu formation and dissolution at the nanoscale is crucial for understanding copper transformation electrochemistry.

**Keywords:** *In-situ* TEM; Liquid Cell TEM; Electrodeposition.

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## High resolution imaging of boron atomic columns in $\text{Nd}_2\text{Fe}_{14}\text{B}$ permanent magnet using electron ptychography

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Aberration correctors have made optical system in scanning transmission electron microscopy a wide-spread tool for material characterization at atomic level. Traditional image resolution was limited by the microscope's optical parameters and the electron probe energy, but this no longer holds for techniques from the coherent diffractive imaging family. An example is an electron ptychography which utilizes information redundancy, obtained from overlapping scanning positions, to image electrostatic potential of weakly scattering specimens. This approach enables reconstruction of the exit electron wave phase as well as the probe aberrations resulting in imaging of the light elements. Conventional ptychographic methodologies were successfully applied in imaging of light elements, yet limitations are set due to thickness of the specimen. Recent developments of reconstruction algorithms focus on mitigating limitations due to material thickness by implementing multislice method, where each slice of the material would satisfy weak phase object approximation. In our case study, performed on  $\text{Nd}_2\text{Fe}_{14}\text{B}$  permanent magnet, we apply electron ptychography to image boron atomic columns and correlate success of ptychographic phase reconstruction with probe propagation through the specimen. Further comments will be stated on the future developments of electron ptychography.

## Regenerating single cells of grapevine cv. Zweiglet into whole plants

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Advances in plant genetic engineering and genome editing have facilitated the study of gene function and the development of improved crops through both genetic engineering techniques and informed selection. While these techniques are well established in small leafy plants such as *Arabidopsis thaliana* and other small crops, they pose a challenge when applied to woody plants such as grapevine.

The transformation of single grapevine cells is attracting increasing interest for both research and breeding purposes. This technique is particularly valuable when it enables the regeneration of single cells into whole plants, as the organisms produced in this way usually exhibit minimal chimerism.

Until recently, the successful regeneration of whole plants from single grapevine cells has proved elusive, with only a handful of cultivars having been effectively regenerated to date. Here we present the first successful regeneration of single cv. Zweigelt grapevine cells into whole plants, along with preliminary data on the effects of the plant growth regulator 6-benzylaminopurine.

## Neuropeptide receptor Y as potential target for specific cancer treatment

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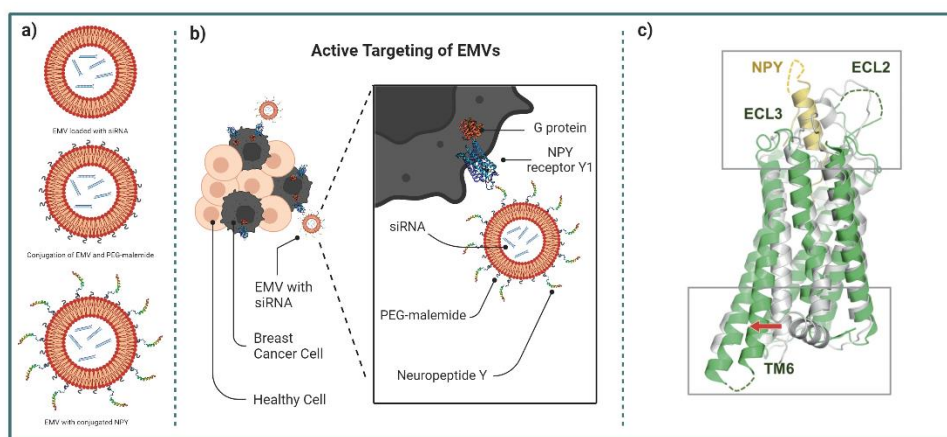
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Neuropeptide Y (NPY), a 36-amino acid peptide, interacts with G protein-coupled receptors (GPCRs) known as NPY receptors (NPYRs), including Y1, Y2, Y4, Y5, and Y6 subtypes [1]. Y1 regulates food intake, heart rate, anxiety, and bone homeostasis, while Y2 influences neurotransmitter release, memory, circadian rhythm, and bone formation. Y4 is involved in feeding regulation, energy homeostasis, colonic transit, and hormone release, primarily in the gastrointestinal tract and brain. Y5, mainly expressed in the central nervous system, regulates food intake, circadian rhythm, and hormone release. The Y6 receptor is active in certain animals [2].

GPCRs, the largest class of cell surface receptors, play roles in cancer development. Over 30% of FDA-approved drugs target GPCRs or related pathways [3]. The targeting of NPYRs with NPY analogs holds immense promise for advancing cancer therapy. By leveraging innovative carriers such as red blood cell ghosts (EMVs) [4], which offer unique advantages with their nontoxicity, biocompatibility, and circulation time, the development of novel NPY analogs gains further momentum. These analogs have the potential to precisely target cancer cells while sparing healthy tissue, thus revolutionizing the efficacy and safety of cancer treatments (Figure 1). We hypothesize that drug-loaded EMVs will be preferentially internalized by cancer cells expressing these receptors, leading to a more selective and effective drug delivery.



**Figure 1.** a) conjugation strategy of EMVs; b) mechanism of active targeting of breast cancer cells; c) NPY Y1 -NPY interaction adapted from Park et al. **2022**, *Nat Commun* 13, 853. Illustration created with BioRender.com

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## Colloidal stability of the ricinoleic-acid functionalized magnetic nanoplatelets in apolar solvents

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Ferrofluids are colloidal dispersions of magnetic nanoparticles in a carrier fluid. Ferrofluids are colloidally stable because the repulsive interaction, induced by the ligands attached to the particles, prevails over the magnetic dipolar attraction between the nanoparticles. At our department ferrofluids and liquid magnets were made by dispersing the DBSA-functionalized magnetic nanoplatelets, based on barium hexaferrite (BHF), in 1-butanol [1]. The colloidal stability of this highly concentrated suspension was achieved through electrostatic repulsion by the double DBSA layer. Such polar dispersions are conductive and cannot be used in an electric field. Obtaining similar dispersions in apolar solvents is difficult, because the long-range electrostatic repulsive interactions, which oppose the long-range magnetic attractive interactions, are absent. Consequently, stable dispersions can be made only by functionalizing the nanoplatelets with large enough ligands that provide sufficiently long-range steric repulsion between the nanoplatelets. Ricinoleic acid is such a surfactant and can therefore be used for dispersing nanoparticles in apolar solvents [2].

In a search for a suitable apolar solvent, we functionalised the hydrothermally synthesised BHF nanoplatelets with ricinoleic acid (BHF-RA) and dispersed them in different apolar solvents. The solvents differed in their dielectric constants and molecular structures. The concentration of platelets in the supernatant was used as a figure of merit.

Among all tested solvents, the BHF-RA dispersions in chloroform exhibited the largest stable fraction of the dispersion (190 mg/mL). The chloroform molecule was the smallest, with a dielectric constant (4.81 at 20 °C) falling within the mid-range among the tested solvents. A downfall of such dispersions is the high volatility of chloroform, which restricts possible applications. In the future, we aim to develop a liquid magnet in an apolar solvent to enable its application in an electric field.

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## Cyanogen adduct of [XeF][AsF<sub>6</sub>] and products thereof

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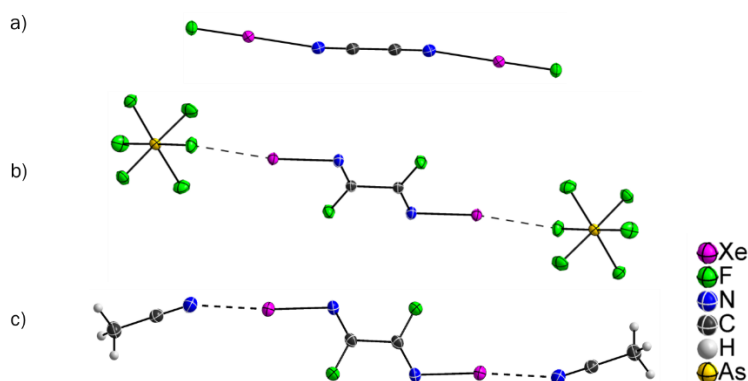
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Nitrogen atoms with sp, sp<sup>2</sup> or sp<sup>3</sup> hybridization are known to form N–Xe<sup>II</sup> bonds in solution and in the solid state [1–3], with sp-hybridized nitrogen atoms being the most commonly used. In all cases, however, only one [XeF]<sup>+</sup> cation was bound to a nitrogen base, leaving open the question of whether more than one Xe<sup>II</sup> atom could be bound to the same molecule. To investigate this possibility, we decided to use the simplest sp-nitrogen base with two binding sites, cyanogen, N≡C–C≡N, which should be stable with respect to the oxidative and fluorinating power of the [XeF]<sup>+</sup> cation due to its high ionization energy.

The reaction of cyanogen with [XeF][AsF<sub>6</sub>] in anhydrous HF at low temperatures yielded the adduct salt [FXeNCCNXeF][AsF<sub>6</sub>]<sub>2</sub> (Figure 1, a), the first example of a nitrogen base *bis*-coordinated with the [XeF]<sup>+</sup> cations. This compound is unstable at room temperature and converts to a [XeNC(F)C(F)NXe][AsF<sub>6</sub>]<sub>2</sub> salt (Figure 1, b), which is the first example of a C=N–Xe bonding modality. Due to the stability of this salt at room temperature and the presence of a polarized Xe<sup>II</sup> atom in the cation, it can be used as a convenient reagent to study the propensity of the N–Xe<sup>II</sup> moiety to form noble-gas bonded adducts with Lewis bases. To explore this, the acetonitrile adduct-cation (Figure 1, c) was synthesized at low temperatures, the structure of which contains a rare example of an N–Xe–N linkage.



**Figure 1.** Novel N–Xe(II) compounds. In a) and c) [AsF<sub>6</sub>]<sup>–</sup> anions are omitted for clarity.

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## A new generation of contact-based antimicrobial biomaterials

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Gold nanoparticles (AuNPs) are used in various applications due to their non-toxicity, stability, and the possibility of functionalization [1,2]. Nanoparticles with surface functionalized with cationic amino acids (arginine) show a strong antibacterial effect through non-specific interactions between guanidines on gold and phosphate groups in the bacterial envelope. Therefore, these particles with a contact-based antimicrobial mechanism exhibit great potential for biomedical purposes [3]. On the other hand, by applying external stimuli (i.e., mechanical deformation, strain, T, voltage), certain materials show piezoelectric properties. Among them is poly-L-lactide (PLLA). During the stretching of PLLA films, the C=O dipole orientation occurs, which, in addition to crystallinity, contributes to piezoelectricity [4]. Here, it is presented the synergy effect of the contact-based antimicrobial mechanism of new gold nanoparticles functionalized with cationic amino acids (arginine, lysine, and histidine) on doped hydroxyapatite as a template and the piezo effect of poly-L-lactide (PLLA) films caused by ultrasound (US) stimulation in order to obtain highly antimicrobial materials. Nanoparticles have been tested against both gram-positive and gram-negative bacteria, and their antimicrobial properties were determined by a series of antimicrobial techniques. The materials showed inhibition of bacterial growth and, in certain cases, a complete bactericidal effect. It has been noticed that when three amino acids is present, particles have better antimicrobial properties than in the case of only one. In the next step, nanoparticles were combined with PLLA films, stimulated using US, and tested for antimicrobial activity. Interesting information about the morphology of the particles using Transmission electron microscopy (TEM) was obtained. Finally, material interactions with HaCaT cells was tested in order to demonstrate the possibility of safe use.

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# Sensor technologies

## Design of experiment methodology to optimize dimethoate hydrolysis and improve fluorescence detection efficiency

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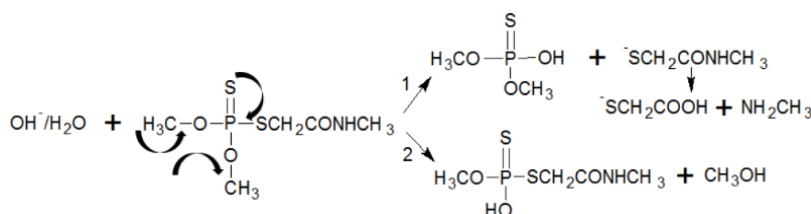
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Organophosphorus pesticides (OPs) pose a significant threat to humans, due to their toxicity, upon both high direct exposure and prolonged low-level exposure, which has been linked to cancer and non-Hodgkin lymphoma [1].

Dimethoate hydrolysed spontaneously in the environment leading to multiple products (figure 1) [2, 3] based on several parameters. Since our dye was sensitive to methylamine we tried to find the optimal hydrolysis conditions with the design of experiment methodology (DoE). We studied how NaOH concentration, temperature and time influence the hydrolysis. Moreover, since NaOH concentrated was degrading our dye, we also included in the DoE the pH at which we have to neutralize after the hydrolysis, to maximize the fluorescence.

Initially, the pesticide undergoes hydrolysis in a NaOH solution, yielding methylamine. Following neutralization, methylamine reacts with the dye in CH<sub>3</sub>CN for 20 minutes. The optimization allows us to achieve an outstanding linear correlation ( $R^2 = 0.999$ ) for dimethoate, spanning concentrations from 7.8 to 292 µg/L and LOD of 3.9 µg/L..



**Figure 3.** Two of the possible hydrolysis pathways of dimethoate<sup>2</sup>

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## Regional Variation of the Vasomotor Zone in Different Postures

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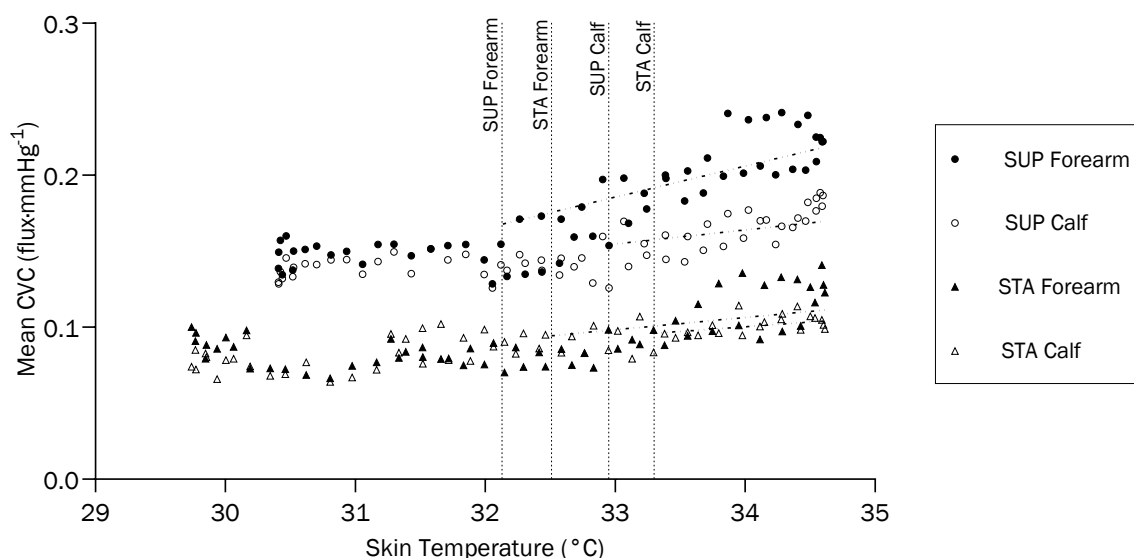
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**Introduction:** In humans, homeothermy is maintained over a wide range of ambient temperatures. Between thermoregulatory responses of sweating and thermogenesis exists the vasomotor zone, where temperature is regulated via vascular control. Within the vasomotor skin blood flow (SkBF) can range from ~0.3 (vasoconstriction) – 8.0 (vasodilation) L·min<sup>-1</sup>. However, blood pressure regulation also influences thermoregulation, affecting vasomotor activity in humans. The aim of the present study was to assess variation in vasomotor activity in differing postures and body regions.

**Methods:** 11 male participants (29.5±6.7 years, 81.1±10.3, 181.5±6.2 cm) attended two sessions, supine (SUP) or standing (STA), where they experienced a 60-min transient thermal exposure (15°C→40°C→15°C). Laser Doppler flowmetry (LDF) was used to non-invasively determine forearm and calf SkBF (CVC, flux·mmHg<sup>-1</sup>), and thermistors measured mean skin temperature (T<sub>sk</sub>) from four sites.

**Results:** Correlation of T<sub>sk</sub> (x-axis) and mean CVC (y-axis) revealed thresholds for vasomotor activity (Figure 1). The vasomotor threshold was reached earlier in the forearm than in the calf, in both SUP (forearm = 32.1 °C, calf = 33.0 °C) and STA (forearm = 32.5 °C, calf = 33.3 °C) conditions. Slope of the forearm in SUP (0.020 flux·mmHg·°C<sup>-1</sup>) was 2x higher than any other limb region or postural condition (SUP Leg = 0.009 flux·mmHg·°C<sup>-1</sup>, STA Arm = 0.008 flux·mmHg·°C<sup>-1</sup>, STA Leg = 0.006 flux·mmHg·°C<sup>-1</sup>).



**Figure 1.** CVC as a function of T<sub>sk</sub>, and thresholds and responses of vasomotor activity, in both limbs and postures.

**Discussion and conclusions:** The relationship between T<sub>sk</sub> and BF<sub>M</sub> differed in varying postural conditions and limbs. The vasomotor threshold occurred at lower T<sub>sk</sub> (~0.9°C) in the forearm regardless of posture. Additionally, the slope of the response (indicating response magnitude) was double that of the leg suggesting a significant autonomic drive to reduce core body temperature. Finally, the postural condition had a smaller influence on vasomotor threshold, but it did influence the individual variability of the response; thermoregulation alone may be more influenced by inter- and intra-individual characteristics.

## Resistive Vibration Exercise with Artificial Gravity: Energy Cost and Muscular Strain

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The European Space Agency (ESA) has embarked on a significant research programme aiming to assess the effectiveness of artificial gravity (AG), induced by a short-arm human centrifuge (SAHC), in mitigating the loss of muscle and bone mass in astronauts for future long-duration space missions. The success of this endeavour hinges on comprehending two pivotal factors: energy cost and muscular strain in our exercises. Therefore, this study compared the energy cost and muscular strain associated with AG to traditional upright exercises.

Fifteen healthy male participants were divided into two groups: Resistive Vibration Exercise (RVE) and Artificial Gravity with Resistive Vibration Exercise (AGRVE). Over the course of 10 training sessions, participants were exposed to vibration training under both normoxic and hypoxic conditions. Various physiological variables were meticulously recorded, including oxygen uptake ( $\text{VO}_2$ ,  $\text{ml}\cdot\text{kg}^{-1}\cdot\text{min}^{-1}$ ), heart rate (HR,  $\text{min}^{-1}$ ), arterial oxyhaemoglobin saturation ( $\text{SpO}_2$ ), and post-exercise energy expenditure (EPEE,  $\text{k}/\text{cal}$ ). Venous blood samples were also taken to assess the levels of creatine kinase (CK) and interleukin-6 (IL-6), reflecting the level of muscular strain.

The results of our study are significant, indicating that the training method (i.e., RVE vs AGRVE) and environment (Hypoxia vs Normoxia) elicited differences within and between groups. Notably, significantly greater  $\text{O}_2$  consumption was observed in the RVE training group compared to the AGRVE group ( $p < 0.05$ ). However, no difference was observed in EPEE ( $p > 0.05$ ) across all conditions. HR displayed significant ( $p < 0.05$ ) differences between groups in light normoxia only (RVE =  $133 \pm 13 \text{ min}^{-1}$ , AGRVE =  $102 \pm 10 \text{ min}^{-1}$ ).

Variations in physiological outcomes between groups are the effect of postural and loading differences, while within-group differences may be attributed to hypoxia. Finally, AG was tolerable however, further investigation is required to assess the appropriate exercise progression.

## Pb(Fe<sub>0.5</sub>Nb<sub>0.5</sub>)O<sub>3</sub>-BiFeO<sub>3</sub> ceramics and thick films for energy storage applications

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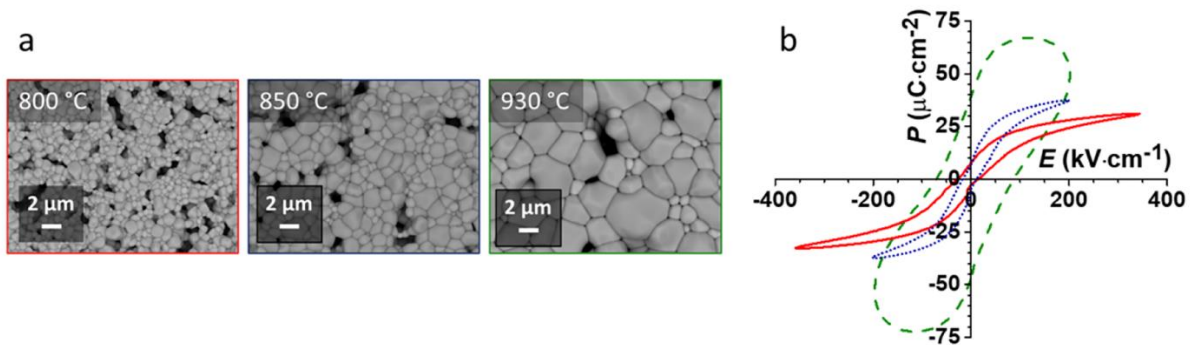
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Energy storage is the ability to collect and store energy for use at another time. Due to their high power density, dielectric capacitors are good energy storage devices for use in pulsed power systems. Among different dielectric materials, the most promising are the materials with slim, pinched polarization versus electric field ( $P$ - $E$ ) hysteresis loops [1]. These properties are achieved in  $(1-x)\text{Pb}(\text{Fe}_{0.5}\text{Nb}_{0.5})\text{O}_3-x\text{BiFeO}_3$  (PFN-100xBFO) solid solutions [2]. Compared to bulk ceramics, thick films withstand higher electric fields and are therefore even more promising for energy storage applications [3].

In this work, we investigated the energy storage properties of PFN-100xBFO ceramics and thick films. PFN-100xBFO ( $x = 0-0.5$ ) powders were prepared by mechanochemical synthesis and sintered at 900 °C or 950 °C for 2 h. The best energy-storage properties were determined for the composition  $x = 0.3$ . The recoverable energy storage density ( $U_{\text{rec}}$ ) and efficiency ( $\eta$ ) values were 1.0 J/cm<sup>3</sup> and 91 % at 70 kV/cm, respectively. After that, thick films of the composition  $x = 0.3$  were screen-printed onto gold-coated Al<sub>2</sub>O<sub>3</sub> substrates. The samples were sintered at 800 °C, 850 °C and 930 °C for 2 h. The  $P$ - $E$  hysteresis loops of the samples and their microstructures are shown in Figure 4. The samples sintered at 800 °C withstood the highest  $E$  and were selected for further investigation of the energy storage properties. The  $U_{\text{rec}}$  value of the PFN-30BFO thick films reached 2.8 J/cm<sup>3</sup> at 400 kV/cm and the  $\eta$  value was ~80 %. The samples were additionally cycled by an  $E$  and survived 10 million cycles. The good energy storage properties and fatigue resistance of the PFN-30BFO thick-film samples show their potential for use in energy storage applications.



**Figure 4.** (a) The SEM microstructures of the surface of the thick films. (b)  $P$ - $E$  hysteresis loops of the thick films annealed at 800 °C (red solid line), 850 °C (blue dotted line) and 930 °C (green dashed line).

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## Behavior of nucleic acids at electrode surfaces: effects of structure and chemical modification

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Electrochemistry links chemical and physical phenomena, and provides us information about the chemical, structural and other changes that can occur on the surface of electrodes. One of the basic conditions to observe these changes is the presence of an electroactive molecule or electroactive group. Nucleic acids are also classified as electroactive molecules, however, very often we use electrochemical labels to increase the sensitivity and selectivity of the nucleic acids detection. In our case we chose to use tags catalyzing hydrogen evolution because they significantly increase the sensitivity of detection. The ability to catalyse hydrogen evolution has been described for, among others, thiopyrimidines. Thiopyrimidines are bases where an oxygen atom has been substituted for a sulphur molecule. The structure of these synthetically modified bases is therefore very similar to natural bases. In this work, we analyzed the behavior of three selected thiopyrimidines (2-thiocytosine, 2-thiothymine and 4-thiothymine). In particular, the aim was to determine the ability of these modified bases to incorporate into the DNA chain using the Primer Extension (PEX) method. This step was verified by denaturing polyacrylamide gel electrophoresis. While 2-thiocytosine was found to be problematic in the sense of its incorporation into DNA, both thiothymines gave full-length products. The behavior of dsDNA with incorporated modified bases was analysed by electrochemical methods, mainly cyclic voltammetry (CV) and differential pulse voltammetry (DPV). When analyzed by DPV, a shift of the potential of the hydrogen evolution peak to less negative values was detected for 2-thiocytosine and 2-thiothymine, which indicates the ability to catalyze hydrogen evolution by such modified DNA. In the course of our experiments, we were also able to confirm that even modified forms of thymine are capable of forming a complex with mercury, as we were able to demonstrate this for both 2-thiothymine and 4-thiothymine.

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I would like to thank my supervisor and my consultant, because they taught me a lot in laboratory and also helped me defend this Master thesis.



## Evaluation of the influence of analog vs digital hardware for electrochemical measurements

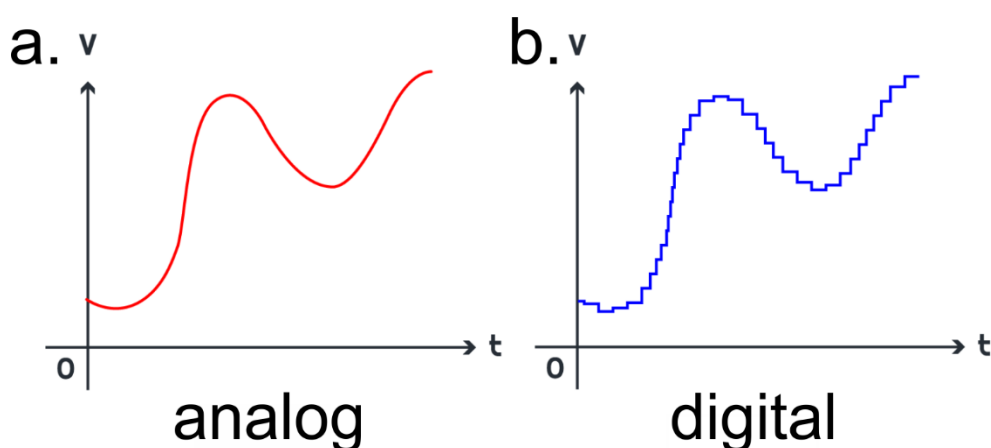
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Modern electrochemical potentiostats have normalized the use of digital hardware. The term digital is referencing the nature of the output signal generated which is discretely quantized in both magnitude and time. Older potentiostats made use of analog hardware which in contrast generated an output signal continuous in both magnitude and time. The ideal digital hardware has a quantization limit approaching zero and is therefore capable of approximating analog hardware but in practice the two waveforms are not the same when looked at higher resolution as illustrated in Fig 1. By utilizing a potentiostat which possesses both analog and digital hardware, cyclic voltammograms for the redox processes of 5 mM hydroquinone in 1 M hydrochloric acid were recorded to check the possibility of variances between the two hardware types and conclusive evidence was noted that the two produce differences that reflect in the CV's. The differences in the voltammograms can be attributed to the charging and discharging processes of the electrolytic double layer, which explain the differences in the recorded output waveforms while not having any influence on the faradaic processes. The results indicate the potential of analog hardware as the norm for electrochemical systems.



**Figure 1.** Comparison between wave functions (exaggerated) generated using a. analog systems b. digital systems

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The above research work was made possible due the Slovenian Research Agency (ARIS), grants P2-0084 (Program Nanostructured Materials), J2-1739 (High Performance Nanostructured Acrylamide Sensors), J2-3051 (SensePMC), PR-09874 (Young Researcher Project). Experiments were performed using a Metrohm VIONIC temporarily loaned by Primalab d.o.o. for trial and feedback.

## Interaction of hypoxic confinement and (in)activity: The effects on sleep quality, mood, and cognition

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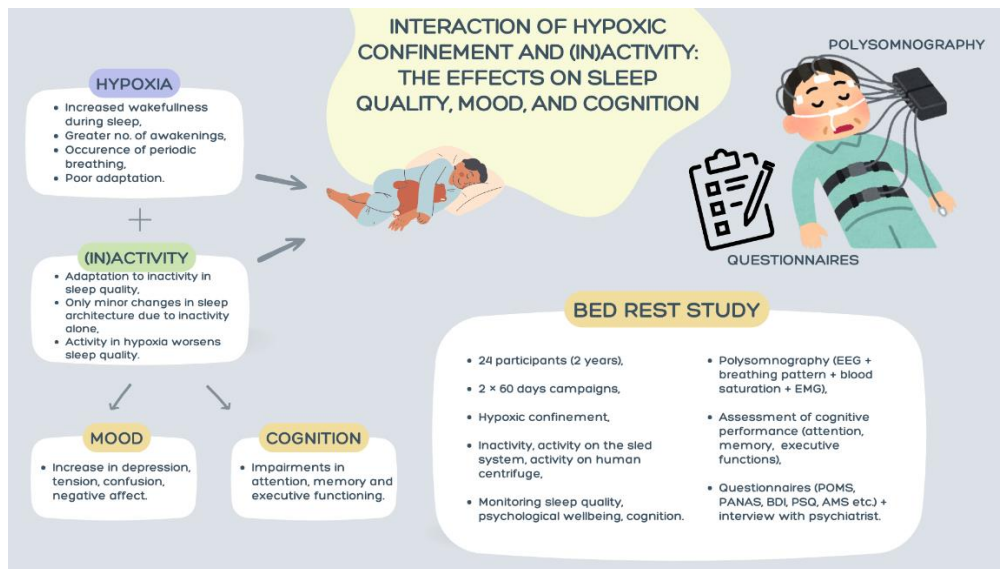


Figure 5. Graphical abstract.

Sleep is a vital process for the body and brain, accounting for 20-40% of our daily 24-hour cycle [1]. Changes in sleep patterns caused by hypoxia and reduced physical activity can lead to cognitive dysfunction and mood deterioration [2, 3]. To evaluate the impact of these conditions on sleep quality, the upcoming 60-day bed rest study will subject participants to hypoxic and weightless conditions to simulate the effects of space travel on the human body. Polysomnography will be used to assess sleep quality, and the study will also evaluate participants' psychological profiles and cognitive functions using various tests and questionnaires. It is hypothesized that participants will experience fragmented sleep architecture, a shift in sleep phases, periodic breathing, exacerbated negative mood, and poorer cognitive performance as a result of these conditions.

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## Lead magnesium niobate-based multicaloric thick-film composites

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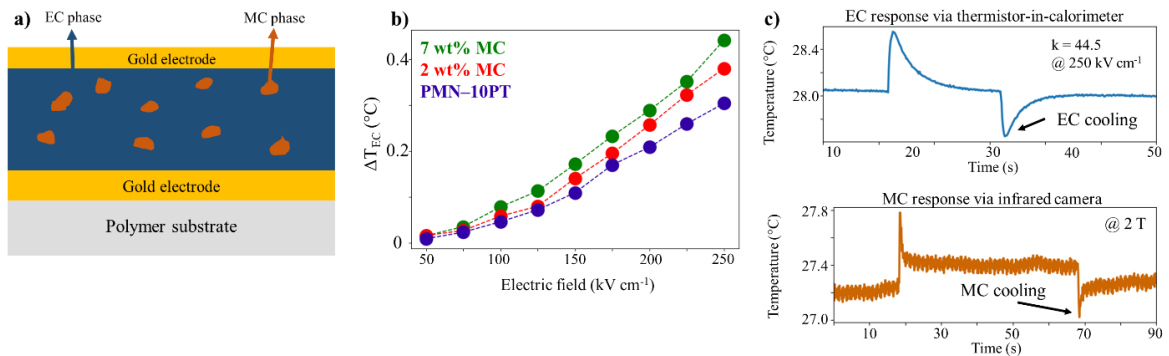
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In recent years, alternatives to vapor compression cooling technologies have received increased attention. Among the most promising options are the ones based on the caloric effects, which are the temperature changes of a material due to an external stimulus, such as an electric or magnetic field. In pursuit of an enhanced caloric output, research has been made on combining different caloric effects, namely the multicaloric effect [1]. However, the combination of electrocaloric (EC) and magnetocaloric (MC) in composite materials remains mostly unexplored. In light of this, using the aerosol deposition (AD) method, we prepared multicaloric composites that combine both EC and MC phases. A suitable EC candidate is  $0.9\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3-0.1\text{PbTiO}_3$  (PMN-10PT), as it shows excellent electrocaloric change,  $\Delta T_{\text{EC}}$ , of up to  $1.5\text{ }^\circ\text{C}$  at room temperature (RT) in thick film form [2]. The MC material, on the other hand, is a La-based MC alloy which shows a temperature change of  $\sim 2.5\text{ }^\circ\text{C}$  at RT [3].

In this work, we prepared AD  $\sim 5\text{ }\mu\text{m}$ -thick films with 2 wt% to 20 wt% MC concentrations on a flexible gold-sputtered polymer substrate (Figure 1a). The films were then annealed at  $400\text{ }^\circ\text{C}$  in argon. Due to the Maxwell-Wagner effect [4], the electrocaloric response (Figure 1b) enhances with increasing amounts of the MC phase, reaching up to  $\Delta T_{\text{EC}} \sim 0.44\text{ }^\circ\text{C}$  at  $250\text{ kV cm}^{-1}$  in the 7 wt% composite. In addition, both EC (measured via thermistor-in-calorimeter) and MC (measured via infrared camera) responses were observed in composites with MC phase as low as 2 wt% (Figure 1c), being the first multicaloric composite thick-film observed at RT. The characterization of the caloric properties of the composites and the influence of the MC phase on the functional properties of prepared composite thick films will be discussed in the contribution.



**Figure 6.** a) Schematic representation of a composite film. b) The electrocaloric output of composites with different amounts of MC phase measured at RT. c) EC response measured using thermistor-in-calorimeter at  $250\text{ kV cm}^{-1}$  and MC (not-corrected data) measured using infrared camera at 2T. The EC response was corrected considering the thermal influences of the setup, the correction factor is  $k = 44.5$ .

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## The effects of 2-weeks resistive vibration exercise with and without artificial gravity on muscle function

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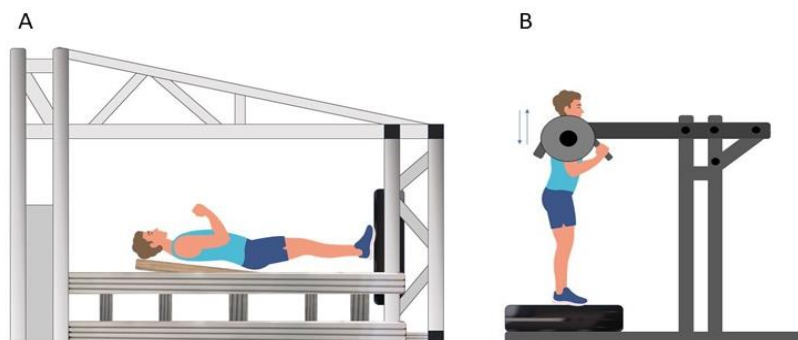
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**INTRODUCTION:** Microgravity negatively affects the musculoskeletal system. Several countermeasures have been explored, but none offer complete protection. Hence, novel strategies warrant investigation. This study investigated the effects of a 2-week daily training protocol using artificial gravity vibration exercise (AGRVE) and upright resistive exercise [(URVE) Figure 1] on muscular function.

**METHODS:** Fifteen male participants (AGRVE = 7; URVE = 8) naïve in vibration and centrifuge training were included in the study. Both groups performed 30 mins of identical training (triple extension squats, squats and calf raise) on a rotational vibration plate at 20hz. Weekly sessions were divided into 3 moderate sessions [4 sets of 8 reps at 40% of 1-repetition maximum (1RM) squat] and 2 light sessions (4 set of 10 reps at 20% of 1RM). Knee and ankle isometric maximal voluntary contraction (iMVC), 8 repetition maximum squat, countermovement jump (CMJ) and body composition were recorded.

**RESULTS:** AGRVE increased iMVC knee extension (KE) and flexion (KF) by 14 and 20% [+34 and +26 NM ( $p=0.0005$ )], respectively. URVE KE and KF were significantly different to AGRVE. Plantar flexion did not change for either group. Dorsi flexion decreased by 20% (-8.70 NM;  $p < 0.0001$ ) with no difference between groups. 8RM increased in both groups [AGRVE = 16%, + 14 kg; URVE = 10%, + 8.75 kg ( $p<0.0001$ )] with no difference between groups. CMJ did not change for either group. Lean mass in the thigh and calf did not change in either group.

**CONCLUSION:** AGRVE improved strength outcomes in the knee more than the RVE. As muscle mass did not change, these strength gains are likely driven by neuromuscular responses. However, the exercise protocol did not yield improvements in ankle isometric maximal voluntary contraction (iMVC). Future investigations into AGRVE should incorporate alternative exercises to effectively target ankle strength.



## Dielectric thick films for use in digital microfluidic thermal switches

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The manufacture of electronic, optical, and mechanical devices is experiencing a continuous trend of miniaturization, making devices smaller and compact, as well as increasing their power density and efficiency. Advances in miniaturization have opened new problems of thermal management in small devices. Potential solutions to improve heat transfer include thermal control devices, one of which is a digital microfluidic thermal switch based on electrowetting on dielectric (EWOD) effect. Such thermal switch requires a multilayer structure (Figure 7a), consisting of a dielectric layer sandwiched between two electrode layers. The dielectric layer has a huge influence on the EWOD effect as well as on the performance of the thermal switch.

In this work, we prepared multilayer structures with three different dielectric thick-film layers and investigated their functional properties. Al<sub>2</sub>O<sub>3</sub> and polyimide P84<sup>®</sup> NT layers were prepared using aerosol deposition method while SU-8 polymer layers were prepared using the spin-coating (Figure 7b). Root-mean square roughness  $R_q$  and dielectric permittivity  $\epsilon'$  values for all layers are gathered in Table 2. According to Young-Lippmann equation for EWOD, Al<sub>2</sub>O<sub>3</sub> dielectric layers are the most appropriate for use in EWOD devices, having the highest  $\epsilon'$  of all three materials ( $\epsilon' \approx 11$ ) and therefore requiring the lowest voltage to achieve certain droplet contact angle. However, the droplet contact angle is influenced by the roughness as well. Therefore, SU-8 layers, which have the lowest  $R_q \approx 4$  nm, were further used to investigate EWOD effect of a distilled water droplet. In Figure 7c, the results of voltage-dependent droplet contact angle measurements are shown. Initial contact angle  $\theta$  is 113°, while the contact angle decreases to 90° at 100 V and to 83° at 175 V. The decrease in the contact angle of water droplets due to increased voltage indicates the potential use of such systems in thermal switch applications.

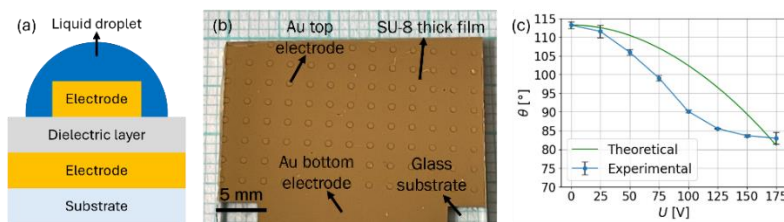


Figure 7: (a) Schematic presentation of multilayer structure. (b) Photograph of SU-8 thick film on glass substrate prepared by spin-coating. (c) Voltage-dependent droplet contact angle of a water droplet.

**Table 2:** The  $R_q$  and  $\epsilon'$  of prepared dielectric thick films.

	Aerosol deposition		Spin-coating
Material	Al <sub>2</sub> O <sub>3</sub>	Polyimide	SU-8
$R_q$ [nm]	40	1400	4
$\epsilon'$ [ ] @ 10 kHz	11	5.5	6.5

## Key role of OH radicals for inactivation of viruses in water

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Water is essential for life, yet it can contain harmful substances and organisms, which cause adverse health effects if consumed. Therefore, purifying our water supply with methods that can effectively reduce hazardous substances is crucial, ensuring that the water we drink is safe. Water treatment methods such as chlorination, filtration or UV radiation have long been the standard methods for water purification, however they all have certain shortcomings, regarding efficiency towards different contaminants, cost, and consumer safety. Advanced oxidation processes, which rely on producing large amounts of chemically reactive species, such as hydroxyl radicals (OH), have been extensively researched for water purification. OH radicals react quickly and indiscriminately against all organic contaminants and could thus be utilized in novel water treatment setups. There are several techniques for producing OH radicals in water. One of which is by utilizing photons in the vacuum ultraviolet (VUV) wavelength, which are energetic enough to break down water molecules into hydrogen and OH radicals. However, their administration to liquid water poses challenges due to their interaction with various substances. Our study addresses this by utilizing vacuum ultraviolet (VUV) radiation generated by an inductively coupled low-pressure plasma device to treat water containing MS2 bacteriophages in a special hermetically sealed chamber with an MgF<sub>2</sub> window facing the plasma source. By varying the applied power, gas inside the chamber, amount of VUV exposure and OH scavengers, we demonstrate that 1) VUV intensity influences the efficiency of virus inactivation, 2) ozone is produced when air is present in the treatment chamber, and that it decomposes to OH radicals in water to contribute to the inactivation of viruses. With optimal treatment parameters, the treatment method could inactivate 9 log<sub>10</sub> viruses in under a minute. This study provides further understanding of the mechanisms of VUV treatment of liquid water.

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