31st May - 2nd June 2023, Kamnik, Slovenia

Jožef
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Institute

turning problems into solutions

BOOK OF ABSTRACTS | 2023

15th Jožef Štefan International Postgraduate School Students' Conference

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Book of abstracts

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Contents

IPS student council

For the second year in a row, the IPS Student Conference was held in the beautiful surroundings of Kamnik. Following two years of virtual editions, last year the conference returned to an in-person format. This incredible experience served as a strong motivation for us to organize the IPSSC once again this year. The conference is organized for students from master's and doctoral programs who are eager to present their work in written and oral forms.

The conference organizing committee has dedicated their efforts throughout the year to ensure that participants feel warmly welcomed, appreciated, and eager to engage in valuable networking opportunities with their fellow colleagues. With a team comprised of passionate and self-motivated individuals, the project never felt like a burden; instead, it provided an opportunity to create something extraordinary and connect with like-minded individuals who share similar experiences. While last year we delved into the realm of science communication, this year we focused on problem-solving skills and critical thinking. The main motto of the 15th IPPSC conference was "Turning Problems into Solutions." As we progress on our PhD journeys, we constantly encounter problems that we strive to solve through our research work. Finding solutions to existing problems is indeed the essence of our profession.

The conference featured a diverse program, including lectures on various topics in line with the main theme. These included talks of invited speakers such as "From Morality to Authenticity: Ethics, Research, and Career Development" by Dr. Tomaž Grušovnik from the Faculty of Education, University of Primorska, and "Should Physicists Make Science or Money - or Both?" by Dr. Mark Pleško from Cosylab. Additionally, Dr. Matija Gatalo from ReCatalyst, KI, presented on "Black Powder" as the heart of hydrogen-powered transport, and Dr. Maya Petek and Tinca Lukan from Young Academy discussed "Choosing the Right Professional Journey after PhD: Exploring Career Options." Furthermore, a round table on the same topic was also held with alumni of the IPS, including Dr. Ita Junkar, who was one of the organizers of the 1st IPSSC, Dr. David Jezeršek, and Dr. Kostja Makarovič, who shared their professional and personal experiences during and after their PhD journeys.

This year, around 70 participants have 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 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.

We would like to express our gratitude to all the students, invited speakers, professors, mentors, members of the scientific committee, and Dean of IPS, Prof. Milena Horvat, as well as the dedicated IPS team consisting of Dr. Aleksander Zidanšek, Sergeja, Maša, and Tadeja. We extend our thanks to our sponsors IPS, JSI, Akrapovič, SCAN Pfeiffer Vacuum, NIB, Salonit Anhovo, Istrabenz plini, ETI, Mikropolo, Primalab, Sanolabor, and Redbull for their support in making this conference free of charge for all participants. Last but not least, we sincerely thank the exceptional organizing team for making this happen.

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

Nina Kuzmić and Žan Gostenčnik,
on behalf of the IPS organizing committee and the IPS Student Council

IPS Dean's words, Prof. Dr. Milena Horvat

IPS student conferences have become traditional and represent one of its the most important annual events. The variety of topics that characterize the annual conference shows the general response of students to the trends and needs of today's society. The theme of this year's conference is *"From problems to solutions",* which is a reflection of today's high-tech needs and increasingly rapid technological development. This is a very ambitious goal, especially considering the early stage of their research and development career. The research work that the students will present at the conference reflects this ambition. Another very important feature of these conferences is the need for clear and understandable communication of research results. This is also a very important part of this process, which can only be effective if excellence, creativity and innovation stand behind the results of scientific work. *In-person* conference is the most effective way of strengthening cooperation within and between different scientific disciplines of the IPS study program and beyond, including different sectors of society.

The challenge of creating an environment where students can pursue excellent international comparative sciences while developing their creative and business skills is one of the major goals of IPS. In cooperation with partner research institutions and industry, we will continue to support all the activities that create the conditions that enable the integration of IPS programs with other Slovenian and foreign universities, academic institutions and industry in order to provide students with the best knowledge and skills they will need in their future career development.

The conceptual design and implementation of IPS conference demanding organizational task was entirely in the hands of the Organizing Committee and the IPS Student Council. IPS and its partners are extremely proud of their commitment and excellent organization. Congratulations to all - those responsible for the organization and those who registered for the conference!

Special thanks also go to the sponsors of the IPS Conference. It is not about the amount of funds provided, but moral support and recognition means more than money can pay. Along with the recognition and acknowledgement, we must not forget the mentors who guide students and help them achieve ambitious goals - the recognition goes to everyone, students, mentors, JSI support staff and partners and founders of the school.

I wish all participants a pleasant gathering and a lot of success in their further research work.

Prof. Dr. Milena Horvat

Ecotechnologies

Total mercury and methylmercury concentrations in blood, urine, and hair of individuals after a monitored intake of tuna fish

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Problem

Fish, particularly predatory fish, can contain significant amounts of methylmercury (MeHg) due to MeHg bioaccumulation and biomagnification through the aquatic food webs. The common assumptions in human health risk assessment are that all mercury present in fish is methylmercury and that 100% of the ingested methylmercury is bioavailable. These assumptions are, however, mostly based on outdated studies with significant limitations, such as very small sample sizes or unrealistic exposure routes, and can lead to an overestimation of the actual risks. Studies investigating the kinetics of MeHg in the human body are similar, with most critical studies performed decades ago.

Solution

With the present study, we aim to reduce the uncertainties in the current human exposure and health risk assessment of MeHg in fish and validate pharmacokinetic models which would enable us to better predict individual internal doses and potential adverse health effects. For this purpose, a realistic exposure scenario was created for 10 volunteers (additional 6 volunteers were recruited as controls), through controlled consumption of tuna steaks and subsequent measurements of total Hg and MeHg in multiple biological samples over a period of 3 months. Each individual in the experimental group was given 5 tuna steaks (steak weight of approximately 300 grams) to consume over 5 consecutive days. Total Hg and MeHg were determined in each steak. Blood, hair, and urine samples were obtained from volunteers before starting the tuna consumption, every other day during tuna consumption, and once a week during 11 post-consumption weeks. A detailed daily record of the way of steak preparation and all foods and drinks consumed at each meal was kept by all subjects. Furthermore, genotyping for single nucleotide polymorphisms previously found associated with Hg kinetics (e.g. APOE, CYP, GPX) was performed and possible correlations with Hg exposure biomarkers were tested.

A green and accurate sampling system for atmospheric pollutants

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Problem

Mercury is among the top pollutants of global relevance. In some areas it is problematic to continuously monitor its atmospheric species due to the lack of infrastructure. The easiest and most efficient way of monitoring in this case is using passive samplers. The advantages of these samplers are i) low cost of manufacturing and operation ii) user-friendliness, iii) low maintenance as they can be left for sampling over long periods of time iv) no requirement for electricity or gasses to function. Unfortunately, there is a large uncertainty contribution related to the sampling uptake rates of passive samplers, thus misinterpreting the degree of pollution of the area. Changes in uptake rates must be corrected according to the meteorological conditions that changed during the sampling period. Even if the meteorological conditions are monitored, the corrections for the sampling rate would not be accurate due to the fact that the sampler are calibrated in laboratory conditions, not in environmental conditions. Long sampling times are also required to ensure that a sufficient mass of mercury is sampled.

Solution

Through this work we propose an alternative sampling technique using gold on silica traps through which we reduced the uncertainty of the sampling rate by using a flow calibrated battery operated micropump. This sampling device offers higher mass loadings and therefore improved detection limits. The battery pack is recharged with solar energy and can work for 6 days without sun, and requires less than 4 hours to charge in dim sunlight. The flow is continuously monitored using a data logger which is used to calculate the sampling flow throughout the whole sampling period, as the flow was calibrated against the voltage. The new sampler has been tested against an online continuous mercury analyser, and 2 samplers which operate on AC power and mass flow controllers.

Mercury isotopes reveal the link between soils and ores in Idrija

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Problem

Idrija is a site with five centuries of mining history. Mercury (Hg) was mined, Hg ore grinded and the process of mercury retorting from ore conducted all at various locations at different points throughout the history. All these activities have heavily contaminated the soils in Idrija and its surroundings. Due to re-emission, soils represent a potential source of Hg to the atmosphere due to volatilization and to aquatic environment due to release from contaminated soil. Hg measurements are very useful for understanding the distribution and transformations of Hg in environmental compartments, but this information is insufficient to draw conclusions about the sources of Hg.

Solution

Using a multi-collector mass spectrometer, which enables the measurement of stable isotopes of Hg, we tried to determine the connection between sources and sinks of Hg in the wider Idrija mine area. It is also known that by measuring stable isotopes, we can also study the occurrence of photochemical transformations, which can have a key influence on the fate of Hg. Hg isotopes were measured ores, rocks and in soils near three smelteries operating at different periods and reference locations. It was discovered that the isotopic composition varies greatly between different mine phases and ores. The heaviest isotopic composition was found in the richest ores and in native elemental Hg. This isotopic composition was corelated well with the soil near the oldest smelteries where Hg is most abundant in heavier isotopes. Reference locations was enriched in light isotopes, originating from litterfall deposition. The soils near newer and more advanced smelteries had the mixture of both fingerprints, indicating that older soil that contained Hg from smelteries got overlaid with layers of new Hg from litterfall deposition.

Validating affordable bicycle-mounted sensors for behaviour change to reduce air pollution

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Problem

Poor ambient air quality, characterised by large temporal and spatial variability, corresponds directly to the society's pollution factor and is significantly influenced by the behaviour of individuals. In Slovenia, residential heating contributes to 75% of the total $PM_{2.5}$ formation, while transport-related emissions account for 8%, respectively [1]. Quantification of air pollutants and development of policies and regulations can contribute to some extent to the reduction of air pollution, while additional inclusion of measures aimed at behavioural change can serve as a powerful decision-making tool for systematic transformations.

Solution

The $PM_{2.5}$ monitoring campaign conducted in Ljubljana, Slovenia, between September and December 2022 is classified as one of the citizen-driven initiatives. A total of 312 bicycle trips were completed to assess the personal exposure of daily commuters. $PM_{2.5}$ data were obtained using real-time, bicycle-mounted optical particle counters (CanAirIO, Sensirion SPS30) whose basic operating principle is based on laser scattering technology. Data acquisition was focused on determining the effects of season and traffic density on $PM_{2.5}$ concentrations, as well as diurnal and local variability in the data. The results indicate that poor micro-conditions are a dominant factor for elevated $PM_{2.5}$ levels in Ljubljana. A city, located in a valley, with regular thermal inversions and weak wind circulation, as well as stable night-time weather conditions, may hinder adequate vertical mixing of air masses, thus amplifying and prolonging the effects of elevated $PM_{2.5}$ concentrations. In addition, the identification of air pollution hot spots, which in Ljubljana are mostly associated with microsites in proximity to major traffic barriers, is crucial for effective regulatory management and improvements in air quality.

This study highlights the importance of mobile monitoring as an applicable and complementary informative-tool to reduce air pollution, as well as a successful citizen initiative to induce behavioural changes to minimise personal $PM_{2.5}$ exposure.

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A simulation of cycling activists affecting change in behavior

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Problem

An important question has plagued urban developers, policymakers, environmental researchers for decades: do activists and promotors of cycling affect change in behaviour with urban dwellers and their exposure to particulate matter (PM)? While this might not be in the forefront of the scientific community, we set out to explore this question in a virtual environment. A simulation with a stochastic model, e.g., agent-based model (ABM), is a simpler and cheaper option. Individuals and their behaviour are simulated in a virtual environment, based only on population and aggregated research data. The authors acknowledge that this is not a substitute for real-world research. Rather, it is an exploration to provide another tool to design better research.

Solution

An ABM was constructed in Netlogo (Figure 1), assessing exposure of 100 individuals to PM. Their actions were governed by inherent probabilities of performing an activity, based on population data, e.g., a ~33% probability of sleeping. Each activity was associated with (1) an intensity level, determining how vigorous an activity is, and how it affects their minute ventilation (amount of air they breathe in one minute), and (2) a pollution level of PM, based on published research. A certain percentage of agents were so called activists, individual agents that prompt other agents to reduce their probability of choosing a car/bus as their mode of transport, rather opting for walking/cycling. Each hour agents select an activity based on the modified probabilities.

Results show that simply increasing the share of activists or their influence does not increase the intake dose of PM, if the concentration of PM is relatively low. When the outdoor concentration of PM increases, the activists play an ever-increasing role in elevating the intake dose of individuals.

These models can be further augmented, enhanced and calibrated based on outcomes of real-world exposure research.
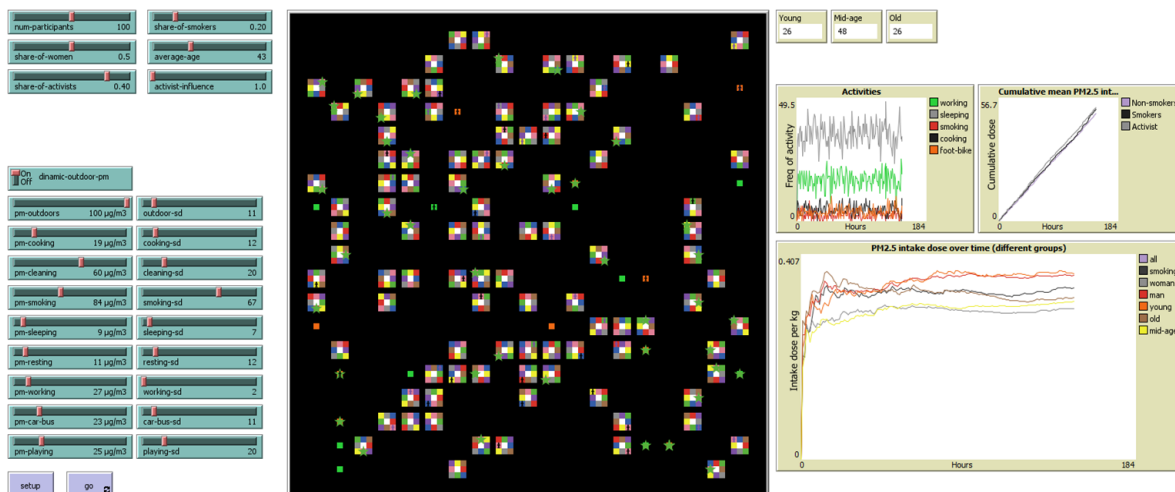
Figure 1: Visualization of the Graphic user interface of the ABM

Biopolymer/Cellulose Nanocrystals Biocomposites: Physicochemical Properties and Biodegradation

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Problem

As a response to global crisis regarding plastic pollution, extensive efforts are being put into providing a suitable alternative with lower negative impact on nature. Alginate and chitosan have the ability to form films and therefore produce lightweight and flexible films that have high potential as packaging materials. Both biopolymers originate from marine biomass and are non-competitive with food supply chain. Originating from biomass, biopolymers are renewable, non-toxic, biocompatible and biodegradable, however their mechanical strength is not yet comparable to commercial plastic foils [1]. Furthermore, while biopolymers are generally degradable in nature, it is unknown whether it is the case for biocomposites.

Solution

To enhance mechanical properties and water barrier, pristine and previously acetylated cellulose nanocrystals (CNCs) were added to alginate and chitosan film forming solutions (FFSs), respectively. The produced films were firstly studied in terms of structure (by means of ATR-FTIR) and properties relevant for packaging materials such as mechanical properties, thermal stability, barrier properties and water contact angle (WCA). Mechanical properties, such as tensile strength (TS) and elongation-at-break (ε) were improved upon incorporation of CNCs in both biopolymer matrices. Chitosan-based films with incorporated acetylated CNCs have also shown to be a better water vapor barrier compared to films based only on chitosan. Upon incorporation of CNCs, WCA increased in all samples, indicating a decrease in hydrophilic nature of the surface. Incorporation of CNCs into the biopolymer FFSs also slightly increased thermal stability of the fabricated films. Finally, to evaluate the end-of-life of such bionanocomposites biodegradability in activated sludge was studied. Biodegradation, measured through respirometry by following the change in partial O_2 pressure in OxiTop® setup, was shown to occur over the course of 72 h and 107 h for chitosan and alginate respectively.

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Deep eutectic solvents as the future of metal recovery

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Problem

The use of lead-acid batteries is widespread for various applications due to their excellent properties. One of their advantages is that 99% of them are recycled, which is an important step towards a circular economy. In the recycling process, for every ton of recycled metallic lead, 100 – 350 kg of secondary lead slag is produced, which still contains up to 22% lead and some other toxic metals such as cadmium and zinc. In order to reduce the amount of this toxic waste and approach the goal of zero waste in the EU, there is a need to develop efficient technologies for the separation of components, which would also provide an additional source of raw materials for the production of new batteries. Several processes have been proposed for the processing of secondary lead slag, but for now they are either low-efficiency or extremely energy-consuming, environmentally unfriendly and uneconomical on an industrial level.

Solution

The solution to the problem is proposed in the development of new hydrometallurgical techniques using deep eutectic solvents, which are environmentally friendly, affordable and often achieve better efficiency and selectivity than conventional leaching agents. For now, the field of application of DES for lead recovery is still poorly researched. On the sample of secondary slag from the company MPI-Reciklaža d.o.o. from Mežica, Slovenia, we thus performed the first test of the efficiency and selectivity of various deep eutectic solvents for leaching lead, which is present in elemental, sulfide and sulfate form. With some combinations of DES, we have achieved more than 85% leaching efficiency, and with the composition of DES itself, we can also influence the selectivity towards other metals present in higher concentrations, such as copper, iron and zinc.

Concentrations of zinc, iron, calcium, magnesium, and potentially toxic elements in food supplements

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Problem

The deficiency of essential elements can negatively affect human health and lead to several modern-life diseases. As a result, there is an increasing demand for high-quality, safe, effective, and highly-bioavailable dietary supplements that can help to compensate for these deficiencies. However, the regulation of dietary supplements currently falls under food law, which has less stringent requirements than drug law. This has resulted in questionable quality and purity of many supplements, raising concerns about their safety and efficacy. The bioavailability of dietary supplements is a critical factor in their effectiveness, as it determines how much of the essential nutrients can be absorbed by the body. The absorption processes of these supplements in the gastrointestinal tract are significantly influenced by the pH value. Negatively charged complexes of elements with low molecular organic ligands are more efficiently absorbed through the intestinal tract by entering epithelial cell membranes in a slightly alkaline physiological environment (pH around 8) such as the small intestine where absorption mainly takes place.

Solution

In this study, we investigated the actual content and purity of zinc, iron, magnesium, and calcium dietary supplements for children and adults in various organic complexes and in a form of inorganic salts. The supplements' total element content was determined using an inductively coupled plasma mass spectrometry technique (ICP-MS) after microwave-assisted digestion of the samples in nitric acid. We also evaluated the potential risk of contamination of supplements with potentially toxic elements (PTEs) such as cadmium, lead, nickel, chromium, and arsenic. The results of this study provided valuable insights into the contents of essential elements in dietary supplements, as well as identified potential risks associated with PTEs contamination. This information can help consumers make informed decisions when selecting dietary supplements to compensate for nutrient deficiencies.

Aluminium can potentiate fluoride-mediated apoptosis in macrophage THP-1 cells

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Problem

Fluoride toxicity is a well-known public health problem, especially in areas where drinking water is fluoridated or naturally enriched with fluoride [1]. The presence of aluminium salts, which are often added during drinking water treatment to remove impurities and improve water quality [2], can lead to the formation of aluminium fluoride complexes. Despite extensive research on the effects of fluoride consumption on human health, little attention has been paid to the effects of aluminium fluoride complexes on specific cells of the human immune system. Macrophage cells play a critical role in the immune system by phagocytosing foreign bacteria and eliminating damaged or infected cells through their specialised pathway of programmed cell death [3]. Chemicals or foreign substances that can inhibit or alter this apoptosis pathway have the potential to affect human health [4]. Therefore, understanding the effect of fluoride and aluminium fluoride complexes on macrophages can help identify potential health risks associated with their consumption.

Solution

The aim of this study was to investigate the effect of fluoride and aluminium fluoride complexes on apoptosis and necrosis in THP-1 macrophages. Cells were treated with standard solutions of (1) fluoride and (2) fluoride and aluminium in a 1 : 1 molar ratio, with concentrations ranging from micromolar to millimolar. Flow cytometry was used to analyse 5×10^5 cells and annexin V/propidium iodide assays were used to detect early-stage apoptosis and late-stage apoptosis/necrosis. The results showed that both fluoride and aluminium fluoride complexes caused a dose-dependent decrease in viability, with aluminium fluoride complexes showing greater potency than fluoride. Even at micromolar concentrations statistically significant differences as compared to the negative control were observed. Although low concentrations do not always lead to significant changes in cellular metabolism, long-term exposure to these species and their cumulative effects may pose a potential health risk.

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Authentication and traceability of fish and seafood using stable isotope and multi-elemental approach

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Problem

Aquatic products are highly desirable since they provide many important components in the daily diet. The expanding commercialisation of products derived from fisheries and aquaculture provides many opportunities for mistreatment and fraud. To avoid and reduce the risks of adulteration and counterfeiting of fish and seafood, the development of analytical techniques, databases, and chemometric approaches is needed.

Solution

This study demonstrates how stable isotopes of light elements (δ^{13}C, δ^{15}N, δ^{34}S, δ^{18}O, δ^2H) and elemental profiles can be used to verify the declared geographical origin of fish and seafood, while also differentiate between organic and conventional fish production in order to prevent or reduce fish and seafood fraud. Comparison between wild and aquaculture samples will be done, where we expect that the farmed fish will have significantly different isotopic signatures compared to wild animals due to the different sources of feed and feeding patterns.

Fish and Seafood authentic database will be established with selection of samples from three different areas (Mediterranean Sea, Atlantic Ocean, and North Sea). While gathering stable isotopes and elemental profiles we encounter many challenges, as aquatic products are affected by many factors (diet, biological characteristics and cultural environments).

Isotopic composition of light elements (δ^{13}C, δ^{15}N and δ^{34}S) in the fish dorsal muscle tissue and seafood soft tissue will be measured by an IsoPrime100 – Vario PYRO Cube Isotope Ratio Mass Spectrometer (IRMS), while the measurements of oxygen (δ^{18}O) isotopic composition in isolated water from the tissue will be determined by IsoPrime MultiFlow system coupled to IRMS. Fish and seafood edible parts and shells will be used for multi-elemental analysis measured with inductively coupled plasma mass spectrometry (ICP-MS).

Combination of multiple methods, selection of correct isotopes and elements for specific purposes, wide sample selection and fitting discrimination methods are necessary to carry out analysis with high classification rate.

Dried blood spots in support of innovative human biomonitoring studies

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Problem

Nowadays the human population is unintentionally exposed to a variety of different compounds from food and the environment, which likely play a role in the development of many chronic diseases. Human biomonitoring (HBM) provides a valuable tool for understanding the magnitude of human exposure from various pathways and sources. Since environmental exposures are dynamic, they require frequent, low-cost, and minimally invasive sampling techniques. Wet blood has been one of the most common biological samples, but its collection is expensive, requires properly trained medical personnel, and suffers from low participant compliance.

Solution

To overcome these limitations, innovative sampling techniques such as dried blood spots (DBS) are being developed to support exposomics research. DBS sampling involves collecting a small volume of blood, from the finger or heel, on filter paper and then drying the samples, which can then be easily transported to a laboratory for analysis. Compared to conventional sampling techniques, DBS collection is simple, effective, and inexpensive. DBS sampling is less invasive and requires a smaller blood volume than venous blood sampling, making it more tolerable for participants, particularly in the paediatric population. However, there is a lack of evidence that DBS sampling is equivalent to conventional blood sampling in HBM studies, especially in suspect screening and non-target screening approaches.

Identification of Biomarkers of Effect for Use in Human Biomonitoring

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Problem

The human population is constantly exposed to chemicals in low doses, some of which can cause adverse health effect after long-term exposure, particularly in cases of exposure to multiple stressors from the environment. Human biomonitoring provides a methodological framework for assessment of exposure to these chemicals and potential health risks. This is achieved by measuring different types of biomarkers in biological samples collected from people living in selected study areas of interest. Biomarkers can be classified as biomarkers of exposure, effect or susceptibility. This work deals with biomarkers of effect measuring molecular and/or cellular alterations which, depending on the magnitude, may be related to a decline in health. These markers should be able to meet specific standards regarding their analytical qualities, relation to the observed effect, ability to characterize the population based on the effect and the data supporting it. This work aims to identify new biomarkers of effect, specifically for use in assessing prenatal neurotoxicity and in the early stages of life.

Solution

Literature currently available and relevant for the topic was first examined. Pollutants with known neurotoxic effects were described, including pesticides, industrial pollutants and metals, briefly presents the concept of exposome, along with some of the most recurring neurotoxicity biomarkers, such as certain enzymes, certain inflammatory factors and neurotrophins, the concept behind Adverse Outcome Pathways is described by outlining their principles and with an example and a short overview of relevant information from the database is presented. The analytical methods to be used later in the process are also listed and include ICP-MS, HPLC-MS, ELISA, ECLIA, SIMOA, genotyping, sequencing and neuropsychological assessment. The initial portion of the work concludes with a brief evaluation of the presented literature as well as suggestions for improvement.

Plant waste as an alternative feedstock for more economical and sustainable lactic acid production

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Problem

Lactic acid is a very important chemical that can be used as a starting material for the sustainable production of a variety of environmentally friendly biochemicals [1]. Reducing the cost of lactic acid production could make these biochemicals and processes more economically viable, which in turn could promote their wider production and use. Most lactic acid is produced by microbial fermentation using crops that are also used for human and animal nutrition, so it is difficult to provide it in sufficient quantity and at a low price [2]. Plant waste (e.g., from agriculture, households, and industry) rich in cellulose would be a much more sustainable and economical alternative.

Solution

Lactic acid bacteria (LAB) are the best known producers of lactic acid. In order for them to grow on plant waste, they must be equipped with enzymes that can degrade cellulose and suitable transporters to import cellulose degradation products. Since there are no lactic acid bacteria that possess cellulases [3], we have used genetic engineering approaches to develop LAB *Lactococcus lactis* that express heterologous cellulases that originate from other cellulolytic bacteria. To mimic the natural cellulolytic bacteria, we have engineered *L. lactis* strains that display cellulases on their cell surface or secrete them into the extracellular environment. We expressed three different cellulases with two different anchors for surface display. We have examined the activity of the heterologously expressed cellulases on the soluble carboxymethylcellulose. Since cellulases also contain a cellulose binding domain, we also evaluated the ability of these cellulases to bind to crystalline cellulose. So far, our results show that functional cellulases can be expressed by the LAB *L. lactis*, which paves the way for the development of bioprocesses to produce lactic acid from plant waste.

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Foodtrack Database: a new Tool for Verifying Food Authenticity and Origin

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Problem

Food fraud practices for economic gain significantly decrease the value of food products and often mislead the consumer (mislabelling, tampering, adulteration), lose their trust and lead to severe economical and public health risks. Robust and sophisticated analytical techniques such as the stable isotopic analysis play a vital role in creating trust and ensuring food quality and traceability throughout the supply chain.

Stable isotopic techniques are one of the most sophisticated and commonly used methods for food authenticity testing when it comes to detection of adulteration, assignment of geographical origin and identification of production mode. However, a common limitation for such techniques is the need for a standardized, readily accessible, and regularly updated stable isotope reference database.

Solution

This presentation deals with developing the FoodTrack database, which includes stable isotope and elemental composition data of products that are most susceptible to fraud: milk and dairy products, argan and olive oil, lamb, truffles, saffron and fish. The database also includes meta-data: annual climatic effects, pedological and geological background of the region of production, type of production and/or diet. The database will be populated with verified data from the literature and authentic samples data to secure food chain traceability and verify the products claims and labelling.

The FoodTrack database has been structured to enable further multivariate data analysis, Geographic Information Systems (GIS) applications, and modelling. Four different ways of evaluating the results will be presented in the FoodTrack web-based tool covering[1]:

(i) FoodTrack data visualization in a graphical mode (maps) that allow the users to see and understand trends, outliers, and patterns in the dataset; (ii) clustering - an unsupervised data mining approach to group samples according to the year and season of production; (iii) discriminant analysis to differentiate food products according to the year, season, and region of production; and (iv) driven soft independent modelling of class analogy (DD-SIMCA) to verify the declaration of samples. These methodologies trace the food supply chain, but do not provide information on some of the decisions that are made based on the data. Thus, a new approach by involving Explainable Machine Learning will be used to classify a given food product and provide an explanation about the prediction that is made. This approach will serve as the basis for further development of isotopic mapping (isoscapes), providing a cost-effective extension to the isotopic dataset approach.

Acknowledgements:

Information and Communication Technologies

Uncovering the Role of News Outlets in the European Twitter Debate

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Problem:

Online debates are a complex environment in which both founded news and unsubstantiated rumours can proliferate. Discussion on online platforms has significant impact on public opinion and may influence people's beliefs and behaviours, sometimes with dangerous consequences for both individuals and society. Moreover, research on online social media showed that users tend to consume information adhering to their beliefs and interact with peers sharing similar viewpoints, reducing the diversity of opinions they are exposed to. Hence, studying the role of news outlets in public debate and how their content is consumed by online users is of primary importance to understand the presence of threats for both individuals and society.
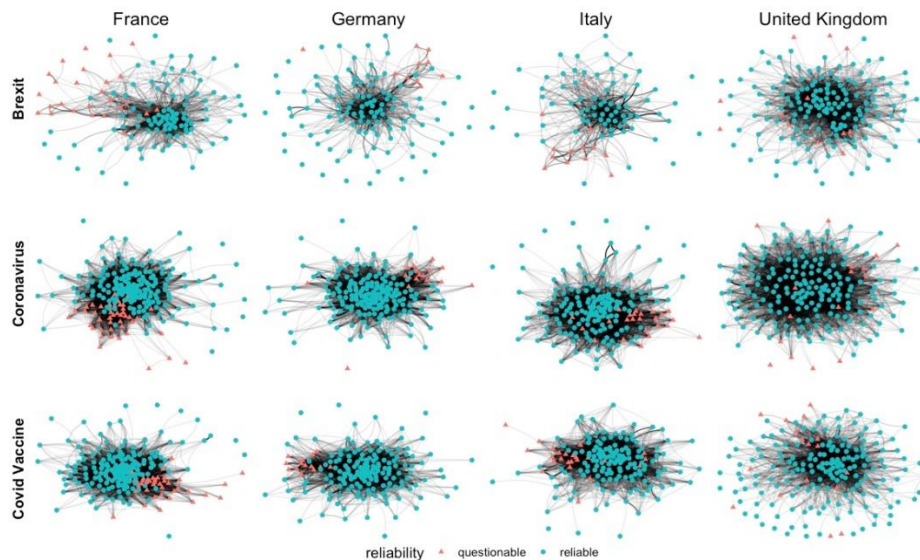
Figure 1: Retweet interaction network of news outlets (nodes). Edges represent similarity in their audience.

Solution:

We study the European debate on Twitter, considering the consumption patterns of over 981k tweets produced by 874 news outlets accounts in four countries over three years (2019-2021). We first perform Topic Modelling to identify most debated topic for Brexit (2019), Coronavirus (2020), and Covid Vaccine (2021), then we study the consumption patterns of news outlets based on source reliability. Finally, based on the interaction patterns of more than 3.2 million users we build similarity networks of news outlets, shown in Figure 1. Our findings show that reliable news outlets tend to dominate the Twitter debate and occupy the core of the network, while questionable outlets tend to be more peripheral. However, some users tend to retweet both questionable and reliable outlets, thus the networks do not have a clear separation between the two types of outlets, and presence of questionable news outlets clusters vary based on country and topic under investigation.

Discovering Exact Equations for Integer Sequences

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Problem

Our research focuses on discovering exact mathematical equations that hold for a given data set of mathematical objects or only a specific subset. Unlike traditional methods in the machine learning subfield called equation discovery that fit measured numerical data up to a certain tolerance of error, our approach tolerates zero error and aims to find exact equations.

Solution

Currently, we are working on discovering equations that govern integer sequences available in The On-Line Encyclopedia of Integer Sequences (OEIS). Given consecutive terms of an integer sequence such as the Fibonacci sequence (0, 1, 1, 2, 3, 5, …) which is governed by the exact recursive equation: $a_n = a_{n-1} + a_{n-2}$ as input, our program outputs recursive equations that hold for all sequence terms. Our assumption that the equation contains only integer values enables us to apply an efficient equation discovery method using solvers of Diophantine equations. In our preliminary experiment, we applied our method to 34371 linear recursive sequences and successfully reconstructed 5783 identically as in the database and 11866 in a more complex form. Our approach is extensible to discovering equations in other data sets containing other mathematical objects. We aim to develop approaches that discover subsets of objects and their corresponding exact equations.

This research has the potential to revolutionize the field of equation discovery by providing exact solutions with zero error tolerance.

Rethinking painting style from the techno-logical perspective: generative art and axiomatic method

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Problem

Artistic style, in a strict sense, is a generative matrix that can be understood with a homology of generative grammar. Style exists not only in its concrete manifestations, such as certain paintings, which cover only the level of articulation, but conceptually subsists as their generative matrix. As an axiomatic system, artistic style is defined by elements of axioms, definitions, syntax, and expressions [1]. The problem is to what extent computers can identify this stylistic generative matrix by analyzing concrete works of art and how their results can serve as a verification process for the concept of style in art theory when generating new works.

Solution

The study uses diffusion models, a type of generative machine learning model that can generate new data based on training data. The models are used to analyze datasets of existing painting styles and generate new variants of these styles (Figure 1 and Figure 2). A variety of Slovene painters were selected to allow comparative analysis. Our results show that the models were able to accurately learn the style of different stylistic paradigms and images very similar to the original works. It implicitly shows how certain theoretical problems and models of artistic style can be verified by their technological solutions in the field of computer science and informatics.
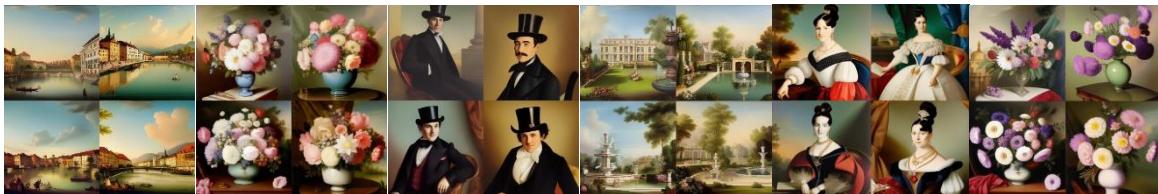
Figure 1: A database of new generated works of a given style.

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Evolution-Guided Equation Discovery

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Problem

Equation discovery is the task of automatically discovering mathematical equations that accurately describe a given set of data or a phenomenon. Typically, this involves identifying relationships between variables from empirical data, with only partial knowledge of the phenomenon. However, current equation discovery algorithms often rely on random sampling, which can lead to lower success rates and longer search times.

Solution

To address this problem, a variational autoencoder can be used to embed similar equations close together in the Euclidean space [1]. This enables more efficient exploration of the space of possible equations using optimization approaches. By defining suitable crossover and mutation operators for an evolutionary algorithm, we can reconstruct equations more quickly and achieve higher success rates. The overview of the approach is shown in Figure 1.
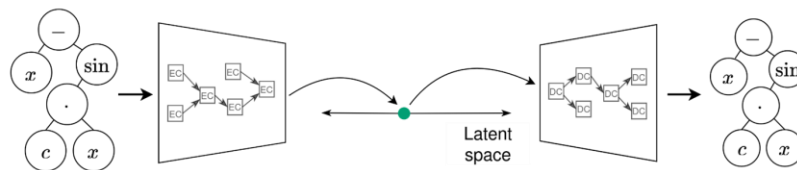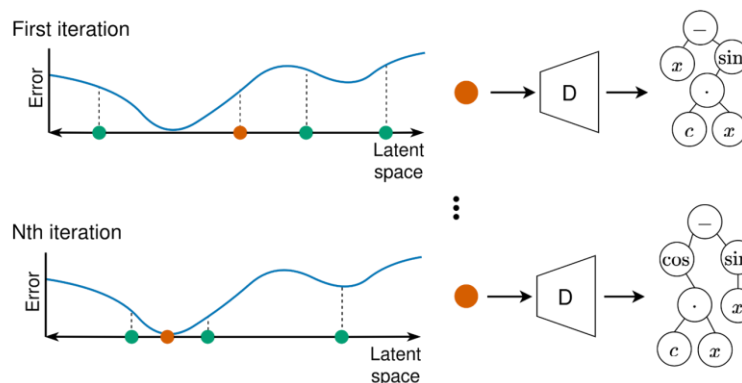
Figure 1. Overview of the exploration process

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Robotised Flattening of a Crumpled Cloth

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Problem

Areas where robots would have to handle fabrics and textiles, e.g., in the textile industry, in the hotel industry, in laundries, etc., are still largely unautomated. The reason for this is the complexity of the actions stemming from the properties of the textiles and the difficulty in accurately determining the condition of textile. As a result, the handling of clothing, fabrics and other textile elements is still done manually, except for the most basic tasks. The properties of textiles, particularly their deformability, self-collision and self-occlusion; and the lack of general approaches in the detection and handling of such materials are prohibitive factors for the robotisation of textile handling. Due to the significant variability of shape and size of flat, non-rigid objects, this challenge cannot be solved with classical algorithms, but requires approaches with advanced deep-learning methods.

Solution

We addressed this challenge by using a vision-to-motion DNN (Deep Neural Network), trained to straighten a single crumpled corner on a rectangular piece of fabric, that was deformed and then flattened in a simulated environment. The neural network was trained to identify a correct grab point at which to grab the simulated fabric and also a correct drop point to which to move the grabbed piece of fabric. For this simplified example, our trained model was able to achieve good results in simulation on a square piece of cloth with the side a=28 cm. Predictions had an average error of 4.4 mm in determining the grab point position and an average error of 4.2 mm in determining the drop point position. The error distribution is shown in (Figure 1a), with the results expressed in pixel values.
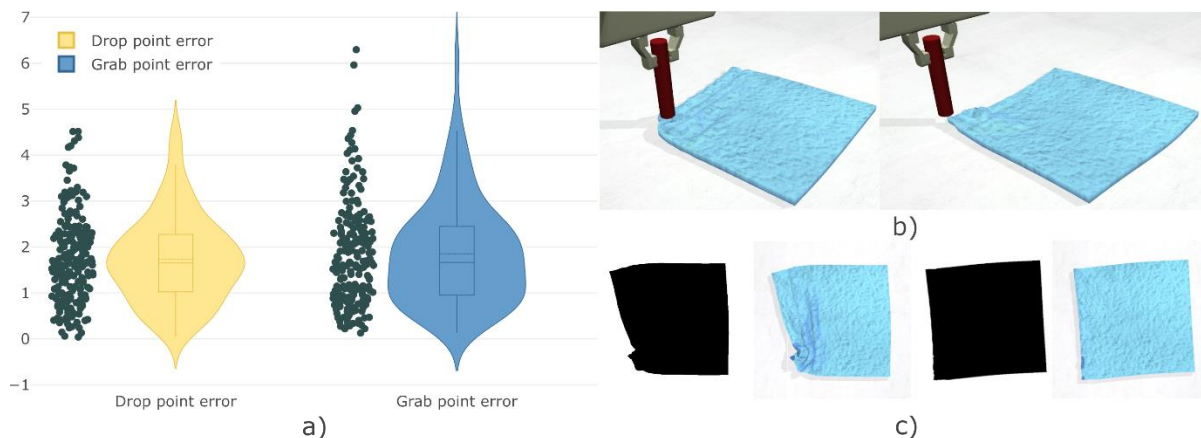
Figure 1. a) Error distribution in grab and drop points on an image of size 256x256 px. b) Robot flattening the cloth based on predicted points. c) Cloth area comparison before and after flattening.

Simulation study of using hydrogen technologies in residential buildings

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Problem

Residential buildings (houses, flats) significantly contribute to the overall energy consumption and use of fossil fuels. A common way to decarbonize residential buildings is to equip them with solar panels, but this does not completely solve the problem. Even if yearly amount of produced electricity exceeds the consumed electricity, there is a problem of mismatch between time profiles of solar power generation and household power consumption. Solar power is widely available in summer time over the day period, while energy consumption increases during winter time due to heating demands (Figure 1).

Solution

One possibility to overcome this challenge is to use hydrogen technologies (electrolysers, fuel cells and hydrogen storage tanks) to convert excess energy to hydrogen and use it later during increased energy demands. In this project we will develop a digital twin of power system, based on solar power enhanced with hydrogen system. We will consider realistic time profiles of solar power generation and power consumption. Digital twin will serve for further techno-economic analysis of the proposed system. Using digital twin the operation of the complete system (energy generation, storage and consumption) will be simulated using different scenarios and sizes of the equipment. The goal is to find optimal solution (optimal system size) that fulfill energy requirement and lowest costs possible.

Figure 1. Total PV and consumed el. energy in moths

Nanosciences and nanotechnologies

Rapid radiation sintering of complex-shaped multi-material ceramic components

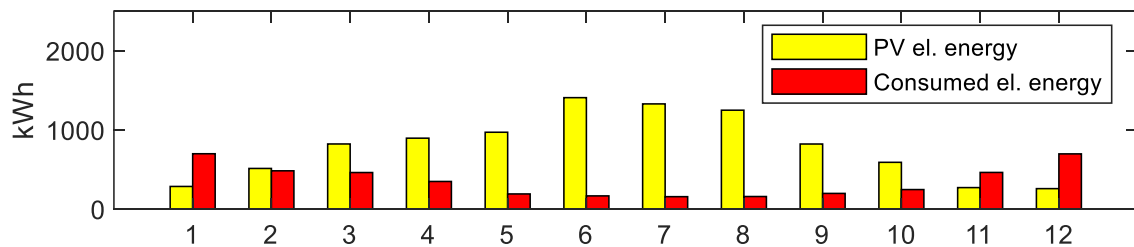**Nikhil Bhootpur[1,2]*, Ipeknaz Özden[1,2]*, Aljaž Iveković[1], Andraž Kocjan[1]**

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Problem

Ceramics are difficult-to-shape materials. Sintering, a crucial time and energy-intensive step, is required for complete consolidation. Dense (pore-free), fine-grained (sub-micron), and homogeneous ceramic microstructures are targeted by controlling densification and grain growth mechanisms, driven by slow solid-state diffusion at high temperatures. In an attempt to reduce sintering time and temperature (energy), applied electrical fields and/or mechanical pressure (e.g., field-assisted, flash, or cold sintering) have been implemented, but with the possibility to sinter simple and mostly planar geometries, limiting the scientific potential of the promising ceramic 3D printing technologies, which can also facilitate multi-scale, multi-material ceramics. It was recently shown how oxide ceramic matrices (e.g., ZrO_2, Al_2O_3) can be infiltrated with sustainable cellulose nanofibers (CNF) [1], [2]. During spark plasma sintering (SPS), CNF in-situ transforms into few-layer graphene (FLG) sheets along the grain boundaries (Figure 1a). FLG pinned the microstructure and provided electrical conductivity, showing promising results for electrochemical applications and electrified catalysis.

Solution

The objective of this work was to translate the concept of CNF-modified ceramic matrices to 3D-printed ceramics, providing a new paradigm for manufacturing ceramics with unprecedented geometries and functionalities. For this purpose, wax-based ceramic feedstocks containing CNF were formulated and rheologically tested. Thermoplastic 3D printing (T3DP) was used to fabricate multimaterial components containing an inner circuit consisting of CNF-ZrO_2 embedded in a ZrO_2 housing (Figure 1b). The role of increased heating rates is studied to provoke the in-situ graphitization of CNF to FLG in the absence of pressure and current in a "pressure-less" SPS sintering set-up based on intense thermal radiation [3]. The latter was shown to be a viable sintering technique to rapidly consolidate 3D-printed monophasic ceramics with fine microstructures [3].

(a)   (b)
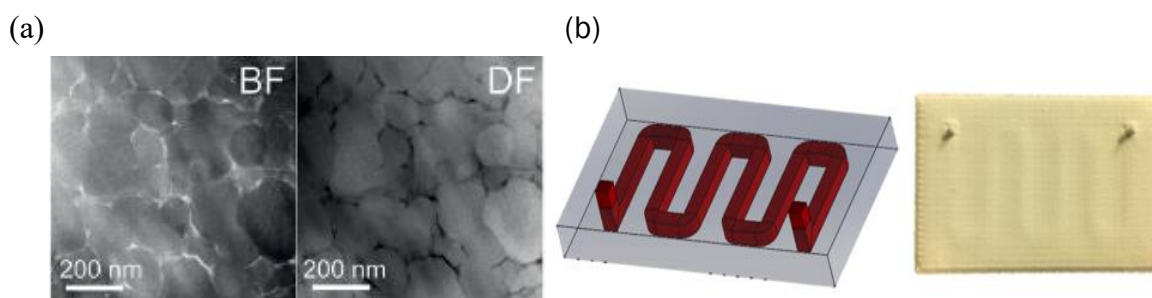
Figure 1: (a) STEM bright field (BF) and dark field (DF) images of SPS sintered CNF-YSZ. The contrast at the ceramic grain boundaries (GBs) in the BF and DF mode is indicative of a continuous intergranular carbon network [1]. (b) Inner circuit of zirconium dioxide (ZrO_2) and carbon nanofibers (CNF) embedded in a zirconium dioxide matrix

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Characterization of polytypic defects in Li$_{3x}$La$_{2/3-x}$TiO$_3$

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Problem

Li$_{3x}$La$_{2/3-x}$TiO$_3$ (LLTO) is one of the most promising materials for applications as a solid electrolyte with excellent bulk ionic conductivity in the range of 10^{-3} S/cm. During the sintering of LLTO with La:Ti ratio of around 0.6 and 20 mol% excess Li, we observed an abundant formation of polytypic lamellae with structural elements of the layered Li$_2$La$_2$Ti$_3$O$_{10}$ phase inside the matrix LLTO grains at lower sintering temperatures. Since the presence of extended defects can have a large influence on the migration of Li$^+$ through the LLTO lattice, it is important to understand the atomic structure of the lamellae, and their further recrystallization to the matrix LLTO.

Solution

We used HAADF-STEM in combination with image simulations based on the multislice method to determine the structure and chemical composition of the lamellae with periodic and non-periodic modulated sequences. The Li$_2$La$_2$Ti$_3$O$_{10}$ phase is composed of (La$_2$Ti$_3$O$_8$)$^{2+}$ pseudo-perovskite blocks (n=2 for the two La layers), separated by (Li$_2$O$_2$)$^{2-}$ layers (Fig. 1a). Intensities of the atomic columns in periodic sequences of the lamellae in experimental images were compared to simulations (inset in Fig. 1a). More commonly, the lamellae have non-periodic modulated structures with different thicknesses of the pseudo-perovskite blocks (higher n values) (Fig. 1b). To reveal the exact composition of the atomic layers in the non-periodic sequence, we prepared models with different exchange rates between the edge La layers next to the Li layers (brightest contrast in the HAADF-STEM image) and the Li layers (inset in Fig. 1b). Based on the results, we determined the degree of ionic exchange between the La layers and neighboring Li layers. We showed that the process further leads to the recrystallization of the lamellae to the matrix LLTO (Fig. 1c) and has an influence on the ionic conductivity of the LLTO phase.
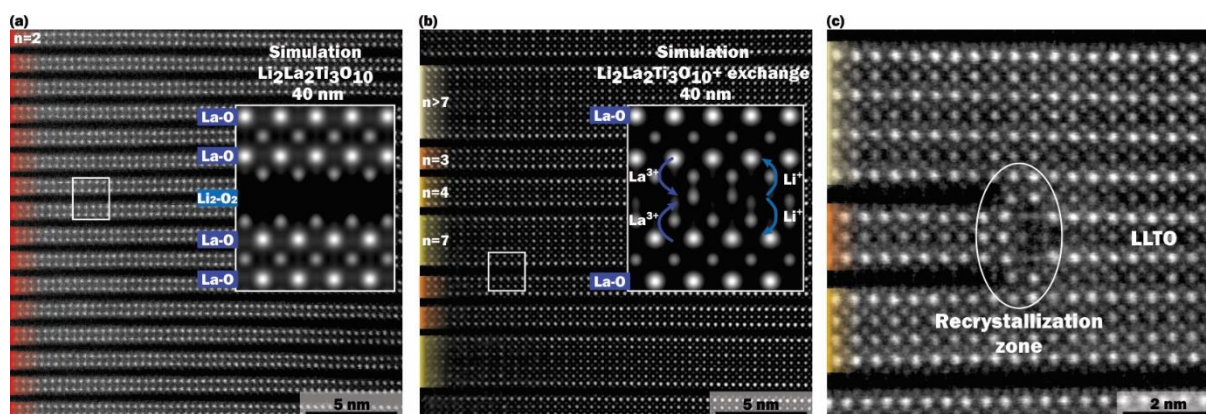

Figure 1. HAADF-STEM images of the (a) periodic and (b) non-periodic sequence. (c) Recrystallization of the non-periodic sequence to tetragonal LLTO.

Synthesis of gold nanoparticles with different shapes and sizes for biomedical applications

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Problem

Over the past few decades, medicine has made impressive progress, but many diseases still lack effective treatments. Fortunately, recent advances in the synthesis of metal nanoparticles have expand their potential applications in different fields, ranging from healthcare research to microelectronics and food packaging [1]. Among the various approaches for exploiting nanotechnology in medicine, gold nanomaterials in particular have been found as the most promising due to their unique optical and physical properties, such as surface plasmon resonance for labelling, imaging, and sensing modalities. Recently, many advancements were made in biomedical applications with better biocompatibility in disease diagnosis and therapeutics [1,2].

Solution

Gold nanoparticles could be functionalized and conjugated with many diverse (macro)molecules, such as polymers, surfactants, ligands, dendrimers, drugs, DNA, RNA, proteins, peptides and oligonucleotides [2]. In frame of medical research, gold nanoparticles offer unique features which can be exploited in electrophoresis, drug delivery, and hyperthermia among others. To explore these applications, we synthesized nanoparticles of different sizes and shapes. Initially, we adjusted the citrate reduction method described by Turkevich in 1951 to synthesize colloidal spherical gold nanoparticles [3]. By reducing chloroauric acid with sodium citrate, we produced nanoparticles with a diameter around 10 nm. Next, we designed synthesis method and synthesized a range of spherical gold nanoparticles with adjustable sizes ranging from 25 to 130 nm. Finally, we synthesized gold nanorods with different aspect ratios using seed-mediated method, which was first described by Nikoobakht and El-Sayed in 2003 [4]. Synthesized nanoparticles were analysed by dynamic light scattering to determine hydrodynamic sizes and by using transmission electron microscope (TEM).

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ALS/FTD-associated C9orf72 C4G2 repeat RNA disrupts phenylalanine tRNA aminoacylation and affects protein production

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Problem

Neurodegenerative diseases have become a leading cause of disability and second most common cause of death just after cardiovascular diseases [1]. This presents a huge burden for health systems and if we consider the aging population this will continue to increase further. Two of severe and highly progressive neurodegenerative diseases are amyotrophic lateral sclerosis (ALS) and frontotemporal dementia (FTD). In the US every year more than 5000 cases of ALS are diagnosed and expected life time after diagnose is 2-5 years. Until now both of the diseases are uncurable and mechanisms that lead to their development are poorly understood. We are focusing on the C9orf72 mutation which is the most common genetic cause of ALS and FTD. Our goal is to detangle the mechanism how this mutation leads to the development of previously mentioned diseases and how translation irregularities are connected with that.

Solution

The C9orf72 gene mutation results in expanded hexanuleotide repeat – GGGGCC. It transcribes in sense (G4C2)n and antisense (C4G2)n direction and leads to the formation of nuclear RNA foci. We determined the interaction partners of less studied antisense transcripts and see which mechanisms are affected by them. These interactions include proteins involved in protein synthesis, cytoskeleton stability and mRNA processing. For the first time we observed the interaction with phenylalanine-tRNA synthetase (FARS). Using several biochemical experiments, we have connected this interaction with impaired translation mechanisms which results in decreased charging of tRNA^{phe} and expression of phenylalanine-rich proteins. This could severely impact normal functioning of cells and potentially lead to the development of the diseases and could present an interesting new target for therapeutic studies.

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Targeted mechanical removal of *Escherichia coli* biofilm

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Problem

In nature, microorganisms exist primarily by attaching to and growing on surfaces [1]. Biofilm formation constitutes an alternative lifestyle in which microorganisms adopt a multicellular behaviour that facilitates and/or prolongs survival in diverse environment. Biofilms represent an important clinical and public health problem. Many bloodstream and urinary tract infections are associated with indwelling medical devices and are simultaneously biofilm associated. In total, it has been estimated that up to 80% of all bacterial infections in humans are biofilm associated [2].

The main problem presented by biofilms is their association with greatly decreased susceptibility to antimicrobial agents [1]. Some medical devices such as catheters can be discarded and replaced; however, other biofilm associated infections may need different approaches. High doses of antibiotics and mechanical removal represent effective ways of biofilm treatment; however, higher doses of antibiotics can be toxic to humans [3] and standard methods of mechanical removal are not feasible in all cases. The lack of effective agents for removal of pathogenic biofilms creates a need for new effective anti-biofilm approaches.

Solution

We propose the use of magnetic nanoparticles that enable the mechanical removal of bacterial biofilm facilitated by exposure to the magnetic field. Biofilms of *Escherichia coli* transformed with a pSEUDO-CP-25-GFP plasmid are established in microtiter plates for 24 h and enable monitoring the effects of magnetic nanoparticles by measuring fluorescence of the green fluorescent protein (GFP) and counting colony forming units (CFU). In preliminary experiments, nanoparticles were capable of removal of 50% of biofilm following 30 min exposure to the magnetic field.
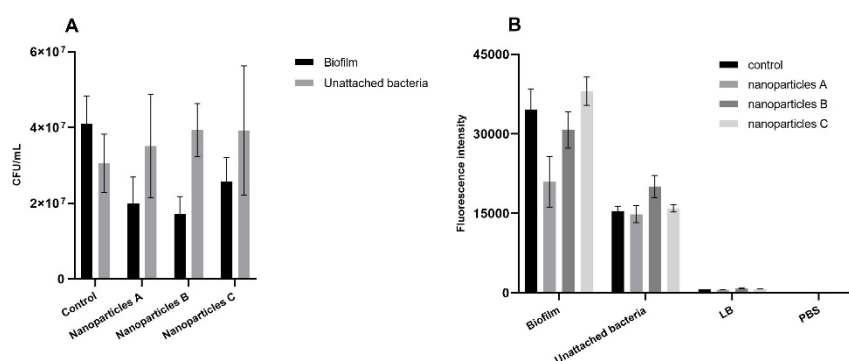
Figure 1: *Mechanical treatment with magnetic nanoparticles causes a significant drop in biofilm-associated bacteria as determined by colony forming units (CFU) count (A) and measurement of fluorescence intensity (B), but no difference in unattached bacteria. Lysogeny broth (LB) medium and phosphate-buffered saline (PBS) represent background fluorescence.*

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siRNA delivery with genipin-polyamines based polymers: characterization, safety, and efficacy

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Problem

Small interfering RNAs (siRNAs) are a promising class of therapeutic nucleic acids. So far, the most widespread approach for their delivery has been complexing them with branched, cationic polymers or neutral carriers. Each approach shows drawbacks, i.e. lack of endosomal escape of neutral carriers and moderate to high toxicity for cationic polyplexes.

Solution

We aimed to assess whether a polyamine/genipin-based scaffold would be suitable for siRNA intracellular delivery, in terms of efficacy, safety, and technical feasibility. RNAs, in nature, are found to be complexed with natural polyamines [1]. Genipin is a natural crosslinker whose glucoside is extracted from the fruits of *Gardenia jasminoides Ellis*. It reacts with primary amines, bridging two different genipin-amines monomers at the end of the process. It's used as chitosan and collagen crosslinker [2]. It possesses a low citytoxicity compared to glutaraldehyde [3], and interesting anti-cancer properties [4]. A novel, biocompatible, non-toxic, polyamines and genipin based polymer, with the addition of glycine as steric modulator, was synthesized (Fig. 1a). The persistence of such polymer, in intracellular environment, was assayed via auto-fluorescence and FITC labeling. Furthermore, FT-IR, coupled with UV-Vis, were used to investigate the polymer formulations and the polyamines and siRNA complexes. Lastly, silencing ability (Fig. 1b) was compared to the state-of-the-art gene carrier, RNAiMAX, and toxicity against various cell lines was evaluated.
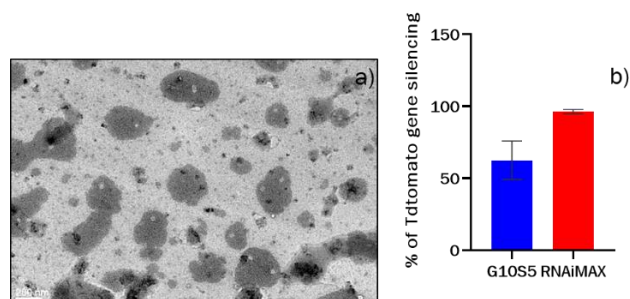
Figure 1. Left, TEM micrography of genipin-polyamines based polymer. Right, its silencing efficacy vs RNAiMAX.

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Chemical stability of barium hexaferrite nanoplatelets

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Problem

Nanoparticles (NPs) are typically less than 100 nanometers in size [1]. They have some distinguished properties with respect to their bulk counterparts. One such property is high chemical reactivity due to their high surface-to-volume ratio [2]. Simultaneously, the NPs decompose or dissolve easier and faster than the coarser particles. The chemical stability is related to the preservation of the NPs` composition and structure under relevant conditions. The dissolution of NPs can lead to release of highly toxic ions when they are composed of toxic metals [3]. To ensure safe use and disposal of NPs, their chemical stability and possible dissolution has to be studied.

Solution

To assess the chemical stability of NPs in bio-systems, there exist quite a few methods, such as electron microscopy combined with microanalytic, surface-sensitive and spectroscopic techniques, and chemical analyses of the dissolved ions. Partial dissolution of the NPs has been already demonstrated by a combination of the X-ray absorption near-edge structure and atomically-resolved scanning transmission electron microscopy [4]. However, in some cases functional properties can be used to measure dissolution of NPs, such as saturation magnetization of magnetic NPs. In addition, dynamic light scattering allows us to follow possible size reduction due to the dissolution, electrokinetic measurements, i.e., zeta potential (ZP) can be used to follow the changes of the surface chemistry in a combination with X-ray photoelectron spectroscopy and infrared spectroscopy.

I am studying the chemical stability of barium hexaferrite (BHF) nanoplatelets (NPLs), the main constituents of advanced materials based on ferromagnetic ferrofluids [5]. I will research the influence of synthesis properties and functionalizing surface ligands on chemical stability of BHF NPLs. Firstly, I will focus on catechols` surface interaction with the BHF NPLs. One of the methods used for measuring the chemical stability of BHF will be ICP-OES, ZP and magnetic properties.

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Chemical analysis of surfaces and thin multilayers

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Problem

In many fields of research, chemical composition of the surface of different samples is very important for their functionality. We need to know both elemental and molecular composition and, sometimes, even oxidative states. In some cases, qualitative analysis is enough while in the others, we also need a quantitative one. Due to the lateral heterogeneity we need to perform imaging of the surface, while differences between surface and bulk require depth profiling to identify individual layers and interfaces. To reveal all this information, we need different analytical methods, with some of them developed completely while others offer a potential for the further improvements and optimization.

Solution

Quantitative elemental analysis as well as determination of oxidative states can be done with the X-ray photoelectron spectroscopy (XPS) which can be used for the depth profiling if equipped with the ion gun. To determine molecular composition, we need a mass spectrometry method such as secondary-ion mass spectrometry (SIMS) (Figure 1) which can be used for imaging and depth profiling. However, SIMS only offers a qualitative and semi-quantitative analysis. The reason behind this is matrix effect causing great differences in the ionization yield depending on the type of the sample, that is substrate/matrix, being analyzed. Matrix effect furthermore limits identification of thin layers during depth profiling. But there are different methods for the reduction of the matrix effect. In our laboratory we use a gas flooding approach, applying both already studied gases such as O_2 and testing new ones such as CO, C_2H_2 and H_2 with the hydrogen posing the greatest potential of them all.
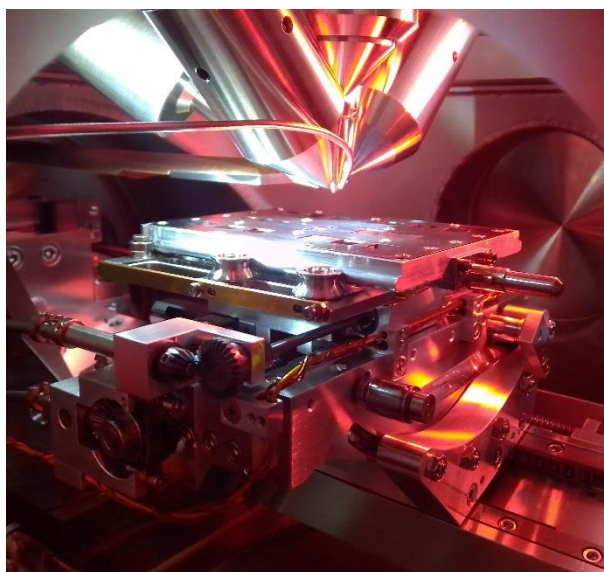

Figure 1. ToF-SIMS instrument

Hydrogen is supposed to be simple

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Problem

We employ density functional theory (DFT) to study hydrogen evolution reaction (HER, $2H^+ \rightarrow H_2$). Its reaction mechanism includes three hydrogen species: hydrated H^+ ion, adsorbed H atom, and H_2 molecule. In order to reliably describe the mechanism, we need to accurately model all three hydrogen species in an aqueous environment. H atom and H_2 molecule are neutral species, and their hydration Gibbs energies are negligible. In contrast, the H^+ cation interacts strongly with water molecules, so its modeling represents a challenge.

Solution

With DFT, one can use different approaches to include an aqueous environment in calculations. We tested two relatively simple methods (Fig. 1): implicit solvent and cluster–continuum models. With the implicit solvent, water is treated as a dielectric continuum without any explicit water molecules. It can effectively describe the hydration of neutral species, but it cannot be used to realistically represent hydrated H^+ cation due to its strong interaction with water molecules. A hybrid cluster–continuum model gives better results because it includes a few explicit water molecules that can form bonds with H^+. This model can also be used on fcc(111) surfaces as an ice-like water bilayer, allowing more reliable calculations of reaction paths for HER. Its transferability to other surface facets is limited due to a symmetry mismatch between the water bilayer and the surface unit cell. Further research is needed to find appropriate models within the DFT framework to describe H^+ cations near electrode surfaces accurately.
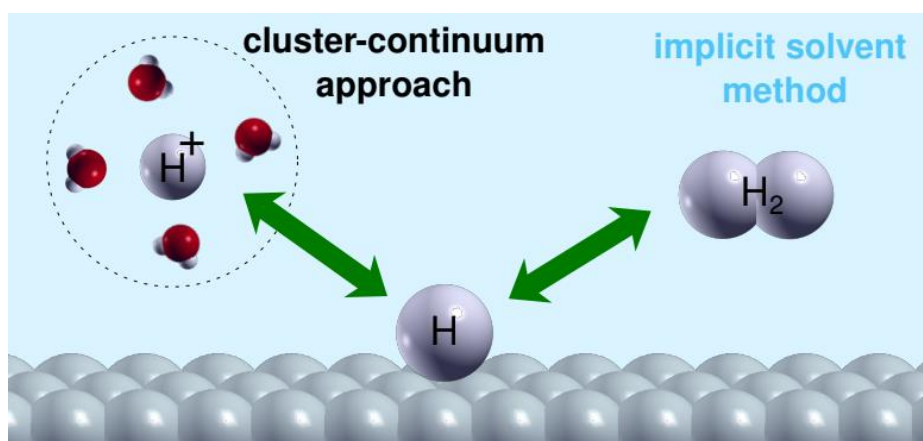

Figure 1. ScheFepresentation of the two approaches for modeling hydrated species near electrode surface.

High Entropy Alloys: A New Promising Type of Material?

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Problem

One of the biggest questions in material science when designing a new material is how to make a material that is hard, tough and strong. It is difficult to design a material with high hardness, toughness, and strength. Especially problematic is the relationship between hardness and toughness. Most hard material are brittle, and tough materials mostly exhibit a low hardness.

Solution

In 2004, a new type of materials called high-entropy alloys has been described in scientific literature that provide a sufficient balance between hardness, toughness, and strength. Such characteristics are a consequence of a high number of different elements (above five) in equimolar proportions present in the material. Therefore, the mixing entropy is higher than in conventional alloys which favors the formation of a solid solution instead of intermetallic phases. The most common structures are face-centered cubic (FCC), body-centered cubic (BCC) or hexagonal-close packed (HCP) structure. Beside the high-entropy effect there are some other unique phenomena, for example lattice distortion due to different atomic radii and sluggish diffusion due to unique structure. Beside superior mechanical properties, high-entropy alloys are resistant against high temperature, corrosion, and oxidation. Specific alloys are even known for their magnetic, electrical, or even superconductive properties.

High-entropy thin films are gaining more popularity since they combine properties of a bulk material and thin films. Plenty of deposition methods exist, however, physical vapor deposition methods are the most common. One of the examples is magnetron sputtering which is already matured technology for the deposition of thin films onto the surface of a substrate.

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The peculiar case of 2-(methylthio)benzimidazole as corrosion inhibitor for copper: A DFT study

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Problem

Corrosion inhibitors are substances that substantially reduce corrosion rate. Computational studies based on density-functional theory (DFT) can provide insight into behavior of inhibitors at the atomic scale. For example, it was shown that mercaptobenzimidazoles bind strongly to surfaces as thiolates [1] (Figure 1a), and strong adsorption is often considered a prerequisite for corrosion inhibition. Along this line of reasoning, the Me-S-BimH molecule (Figure 1a) should not form thiolates because it has its S atom *passivated* with the methyl group (Me). Experiments performed by our experimental team [2] indeed showed that it initially does not protect the copper from corrosion. However, after a few hours of immersion, it becomes an efficient inhibitor. This observation suggests an activated chemical transformation of Me-S-BimH that leads to a strongly adsorbed molecule.

Solution

To solve this puzzle, we investigated using DFT calculations various adsorption modes of Me-S-BimH on Cu(111) that involve the C–S bond cleavages. Our results show that among the two possibilities—i.e., the CS–Me (Figure 1b) and the C–SMe (Figure 1c) cleavages—only the C–SMe cleavage is feasible at room temperature due to the low enough activation energy. The resulting "BimH" molecular fragment (Figure 1d) is strongly adsorbed at Cu(111) and can act as a corrosion inhibitor. However, this reaction requires some time, which explains the experimentally observed delay before the compound starts inhibiting corrosion.
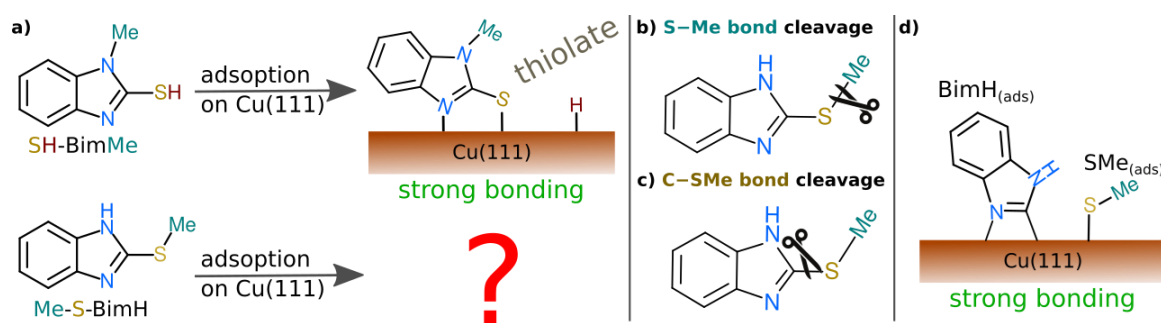
Figure 1. (a) The structure of 2-mercapto-1-methylbenzimidazole (SH-BimMe) and 2-(methylthio)benzimidazole (Me-S-BimH). While the former can easily form a strongly adsorbed thiolate, the latter cannot due to *passivated* S atom. (b,c) Schematic representation of the CS–Me and C–SMe bond cleavages. (d) Adsorption structure after the CS–Me bond is cleaved.

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Epitaxial LiNi$_{0.33}$Mn$_{0.33}$Co$_{0.33}$O$_2$ thin film cathodes as a model system for performance improvement of lithium-ion batteries

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Problem

Lithium-ion batteries have shown great potential for energy storage applications because they provide high energy and power density [1]. However, there is still a need for a deeper understanding of interfacial reactions on the electrode surface that cause degradation and lower battery performance after deep cycling [2]. Lithium-ion batteries can instantly release vast amounts of energy, often resulting in the spontaneous combustion of organic liquid electrolytes, therefore the development of safer lithium-ion batteries is desired for high-power applications.

Solution

Epitaxial thin film cathodes can act as a model system to study intrinsic material properties and interfacial reactions of single-crystalline exposed surfaces [3]. Moreover, epitaxial electrodes can be integrated with solid electrolytes, to develop novel all-solid-state lithium-ion batteries.

Thin films of LiNi$_{0.33}$Mn$_{0.33}$Co$_{0.33}$O$_2$ (NMC 111) were deposited on SrRuO$_3$/0,5%wt Nb-doped SrTiO$_3$ (001) and (110) substrates by pulsed laser deposition from NMC 111 target with 20% lithium excess. High-resolution X-ray diffraction (HRXRD) was conducted, to prove the epitaxial growth and orientation relationship between the film and the substrate. Atomic-resolution transmission electron microscopy (ARTEM) was done to confirm the structural properties of the film. Surfaces of thin films were analyzed with atomic force microscopy for morphology and X-ray photoelectron spectroscopy (XPS) for surface species characterization. For electrochemical characterization, NMC 111 thin films were galvanostatically charged and discharged in the 0.92 – 2.6 V range vs. precycled Li$_4$Ti$_5$O$_{12}$ anode with a current corresponding to 0.1 C-rate. Cells showed stable operation after 100 charge/discharge cycles. Furthermore, we investigated structural and surface changes of lithiated and delithiated NMC 111 epitaxial thin films with *ex-situ* HRXRD and XPS to get more insight into the degradation mechanism of the electrode interface and the bulk single crystal.
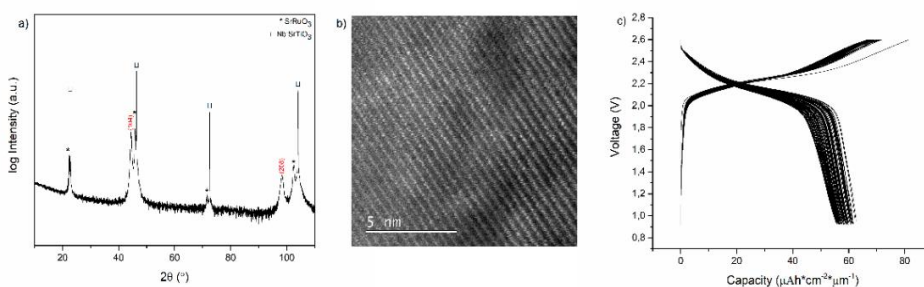
Figure 1. a) XRD pattern of NMC 111 thin film on SrRuO$_3$/Nb:SrTiO$_3$ (001) substrate; b) ARTEM image of NMC 111 thin film; c) Prolonged galvanostatic cycling of NMC 111 thin film vs. bulk Li$_4$Ti$_5$O$_{12}$ anode

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Functional graded tungsten-copper composite as a promising material for future fusion reactors

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Problem

One of the challenges in the realization of fusion reactors is the search for materials that can function under conditions of large and cyclic temperature changes. Tungsten (W) is the material of choice for plasma-facing applications due to its intrinsic properties, such as its high melting point, resistance to erosion and low tritium accumulation, however with constant heating and cooling, tungsten can gradually reduce ductility.

Solution

A composite consisting of W and Cu has been proposed to mitigate the thermal stress, which causes cracks at the surface. The significant difference in melting points does not allow the creation of a strong bond at the W/Cu interface, which is an obstacle to its production. Therefore, several methods should be combined to create such material: the first step is to manufacture a porous W structure, which is infiltrated with molten Cu in the second. To investigate the optimal infiltration conditions, a series of W samples with different porosities were sintered. The variation in pore size was realized by mixing two W powders with different particle sizes. During the subsequent infiltration of molten Cu, the effects of temperature, infiltration time, atmosphere, and W pre-treatment methods on the process were evaluated. The prepared W-Cu composites were characterized in terms of porosity and pore size. It was found that molten Cu infiltration is enhanced in Ar-5%H2 atmosphere in comparison to pure argon; to avoid the gas in the middle of the sample does not prevent the passage of copper, it is best to block the passage of copper through the side surfaces of the sample. The results of the optimal infiltration conditions were applied to the infiltration of additively manufactured W lattice structures fabricated by laser-based powder bed fusion.

Disease detection through biomarkers by using THz spectroscopy

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Problem

More and more patients are suffering from chronic symptoms that progress to serious health conditions that interfere with their daily lives. To detect early signs of diseases, innovative solutions are needed to improve the performance of health monitoring and diagnostics [1]. Over the last few decades, several new methods have been developed to diagnose and monitor disease by analysing biomarkers in body fluids moving in or out of the body [2]. A biomarker is a trait that may be reliably examined and assessed as a sign of different biological processes. Serious illnesses including diabetes, cancer, cardiovascular disease, etc. are predicted using biomarkers. A useful biomarker should be able to reliably identify the disease and forecast its emergence through easy-to-implement monitoring or detection methods [3]. Rapid technological developments are encouraging the use of various sensing devices, including terahertz (THz) spectroscopy.

Solution

THz spectroscopy has recently emerged as an effective biomarker detection technique. The 0.1 THz to 10 THz frequency range of the THz waves matches the vibrational frequencies of various significant biomolecules [4]. Because THz radiation has low energy and does not cause ionization damage to molecules, interest in THz applications in medicine has increased. Intermolecular bonds, such as the hydrogen bonds and the N-H bonds, strongly absorb THz radiation. This means that it is extremely sensitive to little changes, which may indicate the presence of disease. THz light may also explore the molecular structure of substances such as biomarkers within body fluids. In our research, we will focus on the analysis of the noninvasive sources of biomarkers. The THz spectra of various biomarkers present in urine (D -(+)-glucose, urea, uric acid, creatinine) and nipple aspirate fluid (alpha-Tocopherol, gamma-Tocopherol) will be analysed to determine the most appropriate THz frequencies and waveforms to use for health monitoring and diagnostics.

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Advanced Carbon-Based Membranes for The Selective Separation of Molecular Hydrogen

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Problem

The increasing interest in hydrogen economy has led to the development of various approaches for separating molecular hydrogen from different gas mixtures. Membrane-based separation stands out from other existing technologies because of its ability to efficiently separate gasses at the molecular level. Unlike other membranes, carbon-based membranes are still in the early stages of research. Among various forms of carbon, interest in graphene-based membranes sparked when it was demonstrated that a single-layer graphene membrane is impermeable to gases, including helium while being permeable to hydrogen. Since then, many studies were focused on introducing molecular-level pores on graphene sheets and investigating their molecular transport phenomena. However, multistep and multi-approach processing required to synthesize and control the pore density and size limits their large-scale application.

Solution

Recently, plasma-enabled approaches have emerged as promising methods to prepare thin film membranes to separate H_2 from a mixture of gases. Plasma allows the structure-controlled synthesis and fine-tuning of nanostructures, which results in high hydrogen–selectivity and permeability, ease of use, and better scaling potential. Therefore, a low-pressure radio-frequency plasma system will be used for designing structure-controlled carbon-based membranes such as nanowalls, nanotubes, nanocellulose, and bucky paper. The developed materials will be tested for their H_2 separation capabilities. The evaluation will be realized on macroscopic samples, i.e., $1 - 5 cm^2$ disc-shaped membranes sealed with soft material, mounted into a high vacuum system for quantification by quadrupole mass spectrometry. Such structure-controlled membranes will open up new opportunities for effectively separating gases from a hydrogen mixture, which could have potential in hydrogen purification and storage applications.

Crystal structure elucidation of silver(II) sulfates by 3D electron diffraction

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Problem

Currently, single-crystal X-ray diffraction (SCXRD) is the most common technique for routine structural characterization of ordered solids. One of its biggest disadvantages is the need for large enough single crystals (> 1000 μm^3), the preparation of which can be time-consuming or in some cases impossible. Such examples are the antiferromagnetic silver(II) sulfates α-AgSO$_4$ [1], β-AgSO$_4$ [2], and AgSO$_4$·H$_2$O [3], all featuring a rare case of the strongly oxidizing Ag(II) in a non-fluorine environment. Their reported crystal structures were derived from powder X-ray diffraction. However, uncertainty surrounds the structure of α-AgSO$_4$ as it was initially solved in *P−1* space group [1], later redetermined as *C2/c* [4], whereas DFT calculations predicted an *I4$_1$/a* structure [5].

Solution

To resolve these ambiguities, we examined the structures of the silver(II) sulfates using 3D electron diffraction (3D ED). Recent advances in 3D ED place this technique alongside SCXRD in capability, although it is able to extract the diffraction data from crystals several orders of magnitude smaller than SCXRD [6]. Air-sensitive nanocrystalline samples were successfully introduced into a TEM using the newly-developed method for the transfer of reactive samples, and the 3D ED data were collected by continuous rotation method at low temperature. The obtained crystal structures represent a conclusive structural characterization of these intriguing compounds (Figure 1).
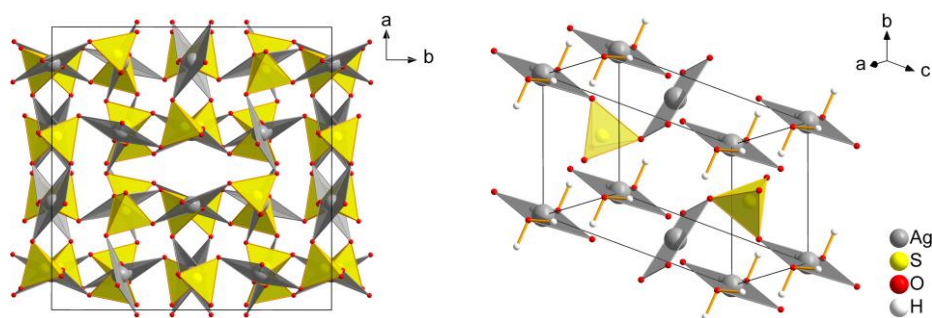

Figure 1. Crystal structures of α-AgSO$_4$ (left) and AgSO$_4$·H$_2$O (right) determined by 3D ED

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Impact of mislocalization on protein interactome of TDP-43

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Problem

TDP-43 is a protein that binds to both DNA and RNA and is typically found in the nucleus. However, in conditions such as amyotrophic lateral sclerosis (ALS) and frontotemporal dementia (FTD), TDP-43 can become mislocalized and accumulate in pathological cytoplasmic protein aggregates, where it becomes the predominant component. In the present study, we investigated the interactome of wild-type TDP-43 and TDP-43 lacking nuclear localization signal (dNLS) mimicking a pathological condition in ALS.

Solution

Using the proximity-dependent biotin identification (BioID) method, followed by mass spectrometry, we identified the protein interactors of wild-type TDP-43 and dNLS-TDP-43. Our results show that wild-type TDP-43 interacts mainly with proteins that are part of the ribonucleoprotein and spliceosome complexes, as well as paraspeckles. In contrast, interactors of mutant TDP-43 (dNLS-TDP-43) are components of cytoplasmic stress granules (SG) and processing bodies (P-bodies). Validation of selected interacting proteins (NONO, SFPQ, FUS, MAML1, PUM1, and ATXN2L) showed that MAML1 is unique TDP-43wt interactor, whereas NONO, SFPQ, and FUS are joint interactors of TDP-43wt and dNLS-TDP-43 and are more abundant in the TDP-43wt fraction. Finally, we found that ATXN2L and PUM1 are unique interactors of mutant TDP-43.

Protein interactions in the presence and absence of NLS resulted in a list of common and unique TDP-43-interacting proteins. Our findings indicate that the development of ALS is associated with loss of regulatory functions related to transcription and/or paraspeckle function, on the one hand, and may be associated with SG and P-bodies due to their enhanced association with mutant dNLS-TDP-43, on the other hand. Furthermore, the newly identified TDP-43-interacting proteins may play a role in the aggregation mechanism or have neuroprotective effects.

MR Imaging and Kinetic Monte Carlo simulation of lithium dendrite growth

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Problem

Although modern lithium-ion batteries are relatively lightweight, have high energy density, and are affordable, they have a significantly lower energy density compared to lithium metal batteries. The use of lithium metal as an anode material in commercial batteries has been hindered by the challenge of lithium dendrite growth, which is not yet fully understood [1]. Dendrites, which are needle-like microstructures that form on the anode during the recharging process, can significantly decrease the battery's capacity. Furthermore, if the dendrites reach the opposite electrode, the battery can short-circuit, creating a thermal runaway and posing a significant safety risk [2]. To prevent dendrite growth in lithium-metal batteries, it is essential to comprehend how the mechanics of electromigration and diffusion affect growth and how nanoscale structural patterns translate into larger scales. Achieving this understanding could be a critical step forward in mitigating dendrite growth.

Solution

While numerous physical models have been developed to simulate the growth of lithium dendrites, we are unaware of any publications where a potential link between the dendrite structural characteristics at various scales has been examined. Our aim is to develop a kinetic Monte Carlo model for modeling microscale lithium dendrite growth, that incorporates Li+ electromigration and diffusion in time-dependent nonuniform electric fields. Simulation results are analyzed and compared with the macroscale images obtained with magnetic resonance imaging (Figure 1). The objective of this research is to establish a connection between the structural features of dendrites at the micro and macroscale levels. Such knowledge could enable the development of safer lithium-metal batteries with reduced or at least more predictable dendritic growth using computationally inexpensive simulations.

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

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Cold sintering of lead-free perovskites

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Problem

Potassium sodium niobate $(K_{0.5}Na_{0.5})NbO_3$ (KNN) and bismuth ferrite $BiFeO_3$ (BFO) are lead-free perovskites that are vastly studied for their use in piezoelectric and magnetoelectric applications, respectively, as promising future devices enabling efficient energy conversion. Since conventional sintering can be challenging, in particular, sintering of KNN which requires about 1100 °C can lead to an inhomogeneous microstructure and the formation of secondary phases, while sintering of BFO requires a narrow temperature range around 800 °C due to possibility of secondary phase formation, these artefacts induced in the material can adversely affect the final ferroelectric properties.

Solution

One of the solutions to overcome the inhomogeneity problems is to use an alternative processing technique. Sintering of ceramics at drastically lower temperatures, i.e., at only 300 °C is possible by the so-called Cold-Sintering Process (CSP) that employs uniaxial pressures up to 600 MPa and the addition of a transient liquid phase.

In our research, we cold sintered KNN and BFO by adding a mixture of the KOH and NaOH hydroxides that form a liquid phase above 170 °C. The analysis of the microstructure with scanning and transmission electron microscopy showed a dense structure, strongly etched and interpenetrated grains, indicating an effective grain-surface melting and sintering of the grains, and strongly deformed lattice with dislocations and faults, all of which significantly affect the materials' properties. Electrical measurements showed that the cold-sintered KNN and BFO have suppressed dielectric and ferroelectric response, while on the other hand, show a lower electrical conductivity, and higher dielectric breakdown strength compared to the conventionally sintered ones. This makes the cold sintering process interesting for tailoring the functional properties of ferroelectrics and potentially creating novel functionalities.

Adducts of xenon difluoride with vanadium(V) oxytrifluoride

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Problem

Xenon difluoride is a good fluoride-ion donor and as such forms many compounds with fluoride acceptors, the most commonly used are strongly Lewis acidic binary pentafluorides, e.g., AsF_5, SbF_5, BiF_5, RuF_5, TaF_5, AuF_5 [1]. Apart from binary fluorides, XeF_2 also forms adducts with transition metal oxyfluorides, however, these compounds are much less explored. Only the adducts of XeF_2 with $CrOF_4$, $MoOF_4$, and WOF_4 have been reported and their crystal structures recently elucidated [2,3]. Although VOF_3 is known to be a relatively good Lewis acid, as evidenced by its interaction with various organic ligands [4] and its propensity to form complex fluoridoanions of varying dimensionality, such as $[VOF_4]^-$, $[VOF_5]^{2-}$, $[V_2O_2F_7]^-$, $[V_2O_2F_8]^{2-}$, $[V_3O_3F_{12}]^{3-}$, etc. [5,6], its interaction with XeF_2 has not been thoroughly investigated. The crystal structures of only two adducts, namely $XeF_2 \cdot VOF_3$ and $XeF_2 \cdot 4VOF_3$, have been determined [6]. However, synthesis of these compounds is challenging owing to the poor solubility of VOF_3 in anhydrous HF, a typical solvent used for the preparation and crystallization of such compounds.

Solution

We have therefore explored the XeF_2–VOF_3 system by employing a novel mechanochemical synthetic approach and by reinvestigation of the thermal reactions. Mechanochemistry enables a rapid and facile synthesis of $XeF_2 \cdot VOF_3$ adduct and a previously unknown $3XeF_2 \cdot 2VOF_3$ compound, both in high purity. Single-crystal growth from the XeF_2 melt enabled us to redetermine the $XeF_2 \cdot VOF_3$ crystal structure and to elucidate the crystal structure of the novel $3XeF_2 \cdot 2VOF_3$ adduct (Figure 1) by low-temperature single-crystal X-ray diffraction.
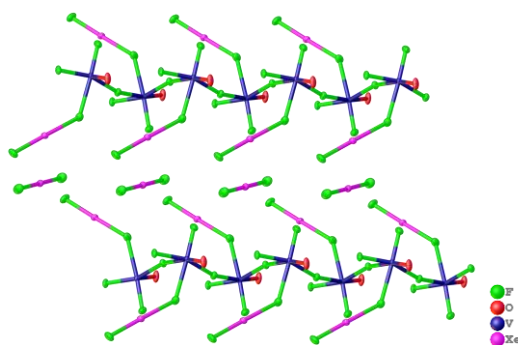

Figure 1. The crystal structure of $3XeF_2 \cdot 2VOF_3$. Thermal ellipsoids are depicted at the 50% probability level.

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LC³ concrete carbonation mechanisms

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Problem

Investigation of carbonation mechanisms of concrete is important from two aspects; carbonation as concrete deterioration processes that can endanger the life of reinforced concrete structures and carbon capture of fresh concrete which causes a slow modification of the concrete structure beneficial for strength and durability improvement. Carbonation mechanisms of limestone and calcined clay cement - LC³ system differs from that of conventional Ordinary Portland cement (OPC) due to the differences in the evolution of phase assembly, the structure of pores and chemistry of pores. Most of the published studies regarding LC³ carbonation deal with carbonation as deterioration process using metakaolin as calcined clay source, while low-grade kaolinite clays, other type of clays or multi-mineral clays as well as CO_2 utilization in concrete are still under investigated.

Solution

The preliminary results of a broader study on CO_2 curing of fresh LC³ concrete will be presented. The study investigated the effect of temperature (10, 20, 60 °C) at constant relative humidity (60 %) and CO_2 concentration (20 %) on the carbonation process, compressive strength and microstructure of CO_2 cured LC³ paste. For the LC³ two type of technical grade clay with different Si/Al ratio (kaolinite and montmorillonite) were used with replacement of clinker with calcined clay and limestone at ranges between 30 and 50 wt. %. Clays were characterized for particle size distribution (PSD) and specific surface area (BET method by gas adsorption). Thermogravimetric analyses (DTA/TG) was used to select the calcination temperature for complete clay dehydroxylation. X-ray powder diffraction (XRD) of calcined clays was carried out to confirm the crystalline phases. To optimise blended cement composition with respect to calcined clays type and gypsum adjustment in LC³ blends isothermal calorimetry was used. Two optimal cement mixtures were selected for further study of CO_2 cured LC³ paste.

Turning CO_2 into useful fuels by catalysis

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Problem : CO_2 emission and its effects

CO_2 is one of the major green-house gases and as of recent reports, the amount of CO_2 has reached the level of ~420ppm according to Mauna Loa Observatory (MLO), Hawaii[1]. In addition, the Earth's temperature rise over the last 200 years has been 0.12˚C per decade[2]. To counteract this problem, one possible solution is to reduce CO_2 into useful fuels like CO, CH_4, HCOO-, etc.[3]. However, CO_2 being a very stable molecule possesses high C=O bond dissociation energy equating to ~750kJ/mol[4]. This makes CO_2 reduction reaction (CO2RR) require high input energy which makes the overall process a highly energy intensive procedure.

Solution : Heterogeneous electrocatalysis

Heterogeneous electrocatalysis is one of the practical answers to the above-mentioned problem. In this work $BiOCl/g$-C_3N_4 nanocomposites were synthesized and tested for CO2RR. The nanocomposites were tested in a gas-tight electrochemical cell connected to an online Gas Chromatography analyzer. The liquid products were analyzed by an Ionic Chromatography analyzer. The Faradaic Efficiencies accounted for 70% - 77% of formate production for the different composites and in particular 52.1% $BiOCl/g$-C_3N_4 formed 259 ppm of formate as compared to 231 ppm by the pristine BiOCl.

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Alkali Activation of Waste Refractory Materials

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Problem

A circular economy aims to minimize waste and the consumption of natural resources. It focuses on the development and use of products that can be reused, repaired, and recycled to create a closed loop of materials and resources. This approach is becoming increasingly important in light of climate change. The building and civil engineering industry is responsible for 40% of global emissions.

Solution

The development and production of environmentally friendly materials such as alkali-activated materials (AAMs) is an important technique to reduce the carbon footprint and increase the recycling rate of waste materials. AAMs have the potential to replace conventional building materials such as cement, concrete and ceramics. This is due to lower energy consumption during synthesis (below 100 °C) and short curing time (a few hours to a few days), which have a positive impact on the product price. Another key benefit of AAMs is that they can be made from waste materials containing sufficient amounts of amorphous silicon and aluminium, whereas conventional building and civil engineering products typically rely on raw materials. AAMs are formed by activating a source of alumina and silica, such as fly ash, slag, or metakaolin, with an alkali activator, such as hydroxides or liquid alkali silicates. In the study, waste refractory material was used as a precursor, which was alkali activated with Na-water glass and cured at 70 °C for 24 h. The aim of the study was to assess refractory material regarding its usefulness as a fire-resistant material, also after alkali activation. Therefore, the precursor and AAM were treated at elevated temperatures (T0, 250, 500, 750, and 1000 °C) (Figure 1). The samples were analysed by SEM, EDXS, XRF, XRD, FTIR and MIP to evaluate the influence of thermal treatment on the material properties.
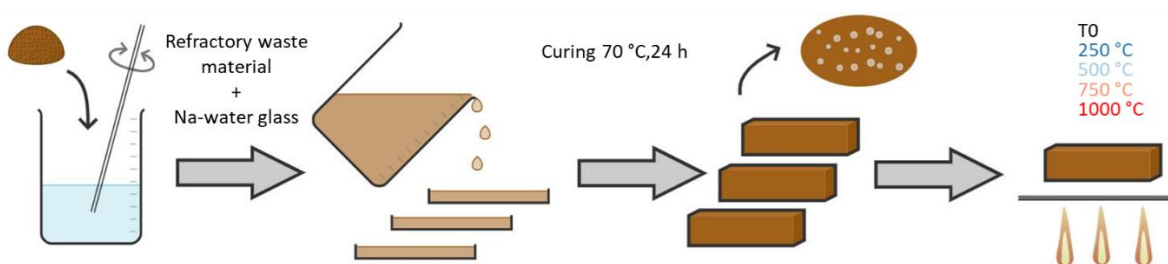

Figure 1: The process of making AAMs from waste refractory materials.

Mechanochemistry of noble-gas compounds

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Problem

The field of noble-gas chemistry has expanded considerably since the synthesis of the first xenon compound, revealing new and fascinating chemical reactivity of "inert gases" [1]. However, to probe reactivity of such compounds, considerable technical and chemical requirements such as metal vacuum line for handling suitable, yet highly hazardous solvents (anhydrous HF, bromine(V) fluoride) [1,2], reactive passivation gases (fluorine or chlorine trifluoride), custom-built vessels and skilled personnel are required. This is currently hampering the progress in this rather exotic field and limiting it to only a few specialized laboratories worldwide.

Solution

In this work, we employed selected reactions with XeF_2 [3] and XeF_4 [4], to demonstrate that mechanochemistry [5] provides a suitable and convenient synthetic route to a variety of noble-gas compounds (Figure 1), without the need for a specialized vacuum line, F_2 gas, and hazardous solvents. Furthermore, we show that in some cases mechanochemistry provides a faster and more selective route for the synthesis of compounds that are otherwise difficult to obtain as pure phases using established synthetic methods. Thus, the simplicity of the developed mechanochemical approach could enable the investigation of noble-gas chemistry by nonspecialized laboratories.
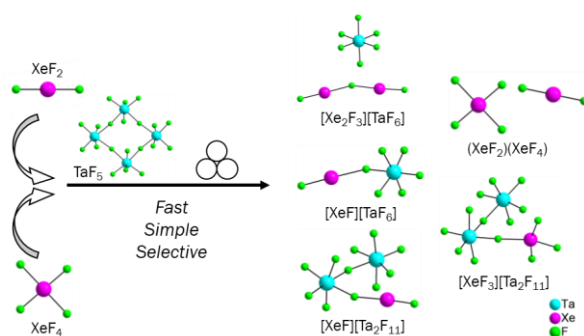

Figure 1. Mechanochemistry enables convenient synthesis of a variety of noble-gas compounds.

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Sensor technologies

Mechanochemical synthesis of selected alkali metal fluoridoargentates(II) and their structural and magnetic characterisation

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Problem

Alkali metal fluoridoargentates(II), $MAgF_3$ (M = Na, K, Rb and Cs), have recently attracted interest due to their electronic and structural similarities to oxocuprates [1]. In addition, these phases are also predicted to exhibit low-dimensional magnetic properties [2]. $MAgF_3$ phases adopt a distorted perovskite structure where the size of M determines the level of distortion: $KAgF_3$ adopts an orthorhombic structure while $CsAgF_3$ crystallises in a tetragonal crystal structure. Despite the high interest, studies on these compounds are scarce. Current synthetic techniques require either long annealing times and high temperatures or sophisticated two-step synthesis procedures involving anhydrous hydrogen fluoride [3–5]. Moreover, these complex procedures lead to partial reduction of Ag^{2+} to Ag^+, which often results in unidentified magnetic secondary phases, making the interpretation of magnetic results particularly difficult [3]. A single-step, low-temperature synthetic method for the preparation of alkali metal fluoridoargentates(II), leading to phase-pure samples, is therefore a prerequisite for understanding their magnetic–structural relationships.

Solution

In this work, we demonstrate that mechanochemistry can be employed to prepare high-purity $MAgF_3$ (M = K and Cs) phases in one step and at room temperature, after only three hours of milling. Our preliminary structural data for the $KAgF_3$ phase is in good agreement with the literature reports, however, our magnetic susceptibility measurements show only one transition, which is in contrast with the previously reported results [3]. Furthermore, $CsAgF_3$ was prepared for the first time using mechanochemistry, and it contains only small amounts of diamagnetic AgF, allowing the first study of its magnetic properties. Moreover, our preliminary laboratory PXRD data supports the previously proposed tetragonal crystal structure with the $I4/mcm$ space group [6].

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Immobilization of the biological recognition elements for the sensitive and selective electrochemical immunosensing

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Problem

Despite high specificity, sensitivity, simple operation, and usually minimal sample pre-treatment the bio-affinity electrochemical immunosensors have not reached their potential in real clinical practice. The main obstacle in the construction of such a device is the immobilization of biological recognition elements on the surface of the supporting electrode. Their orientation, conformational stability, and activity after immobilization determine the sensitivity, stability, and longevity of an immunosensor. This is especially important in the case of antibodies as the biorecognition element, which can be immobilized using one of two ways: via direct adsorption or using site-directed protocols. Direct adsorption has the advantage of being the simplest method but it results in random protein orientation, causing low stability and protein denaturation [1].

Solution

Problems caused by the random adsorption of biomolecules can be overcome with the use of site-directed immobilization. To achieve this a myriad of different methods have been used, with Fc binding proteins (protein A, protein G), antibody fragments, and immobilization via the oxidized oligosaccharide moiety being the most common. This way antigen-binding regions of an antibody will be oriented toward the analyte improving the sensitivity and selectivity of the sensor. The choice of a particular method depends on the goals of the desired system [2, 3]. Here we present several possible approaches for the successful immobilization of the biological recognition elements, demonstrating selective and sensitive analytical performance toward chosen model analyte, i.e., SARS-CoV-2 Spike S1 protein.

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Energy storage properties in Na$_{0.5}$Bi$_{0.5}$TiO$_3$-based ceramics

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Problem

Ferroelectric materials are characterized by a polarization-electric field hysteresis loop (Figure 1a), indicating switching of spontaneous and induced electrical dipoles with an applied electric field. The switchable remanent charges can be exploited as information storage in memory devices [1]. When polarization saturation with electric field is high, but remanent polarization at zero field approaches zero (as is the case in relaxor ferroelectrics; Figure 1b), the difference in the polarization can be used to manipulate and store charges. This property, along with the high-power densities (fast charge and discharge cycles) and limited degradation, makes ferroic materials good candidates for energy-storage devices. However, drawbacks like low dielectric breakdown strength (BDS), low P$_s$ and induced P$_r$ in lead-free ferroics, as well as scalability issues, limits their efficiency.

Solution

Our goal is to design a suitable lead-free relaxor ferroelectric based on sodium bismuth titanate, Na$_{0.5}$Bi$_{0.5}$TiO$_3$ (NBT). While pure NBT possesses a high P$_r$ (38 μC/cm^2) and high coercive field, its relaxor behaviour observed only at higher temperatures, as well as a large leakage current [2]. Creating solid solutions or doping are considered good methods to tailor its properties. Thus, our aim is to induce a relaxor-like behaviour by (1) producing solid solutions with a cubic perovskite, namely, SrTiO$_3$ (ST), and (2) by creating local charge disorder by ionic doping with tin. We synthesized and investigated the properties of NBT–0.6ST composition with and without the dopant. The ceramics shows a decreased P$_r$ at room temperature, and in the case of Sn doping an increased P$_s$. The BDS was decreased, which could be due to porosity in the ceramics. In light of this, the balance between the breakdown field, energy storage density, and resistivity can still be optimized through the variation of ST in (1-x)NBT-xST, by variations in doping, and by microstructure control.
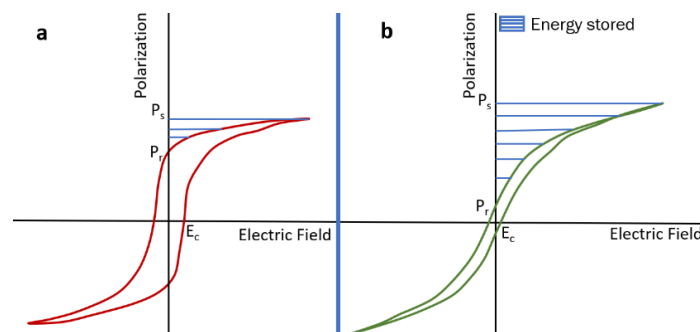
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Development of an Electrochemical Genosensor for the Detection of Hop Disease

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Problem

Hops are of economic importance because of their specific secondary metabolites, which are essential ingredients in the brewing and pharmaceutical industries. Hop diseases, particularly those caused by the Citrus Bark Cracking Viroid (CBCVd), can be very damaging to crops and result in devastating economic losses.

CBCVd is the most aggressive viroid for hops and causes severe symptoms such as dry root rot, plant stunting, and wilt 3-5 years after infection. Viroids are usually detected by conventional molecular biology methods such as polymerase chain reaction (PCR) and enzymatic immunoassays. These techniques are the gold standard with good detection limits and high precision, but they are laborious, time-consuming, and require specialized personnel and facilities.

Solution

Electrochemical genosensors are a novel, straightforward alternative to classical pathogen detection; they combine a biological recognition agent and a transducer to convert the molecular recognition event into a measurable signal. These sensors are fabricated by modifying the electrode surface and immobilizing the biorecognition probe, while the target gene sequence is detected by DNA hybridization. The amount of probe immobilized on the electrode surface should be optimized to enable efficient hybridization while maintaining the desired electrical properties of the transducer. Electrochemical genosensing can be improved by using signal enhancement materials or amplification strategies to increase sensitivity and specificity.

The idea behind the sensor developed in this project is a simple but sensitive setup that allows swift detection of CBCVd in samples of total RNA extracted from hops. The sensor was constructed with an initial layer of streptavidin agarose, followed by the introduction of a biotinylated capture probe that hybridizes with the target analyte, and a final layer of glycine to cover the remaining non-specific binding sites on the sensor surface.

Acknowledgments:

Preparation of Al$_2$O$_3$/Al composite thick films via aerosol deposition

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Problem

With the development of the electronics industry, small high-performance components that can perform multiple functions have been receiving increased attention [1]. For example, Al$_2$O$_3$ is a low-cost mechanically stable and chemically inert material that is already used in electronics devices as a protective and/or an electrically insulating layer [2, 3]. In light of this, it is highly desirable to expand the applications of Al$_2$O$_3$-based materials, such as for large-capacitance applications, for example, embedded capacitors [4]. However, in such cases, the low dielectric permittivity of Al$_2$O$_3$ ($\varepsilon_{Al2O3} \sim 10$) is a limiting factor. Therefore, a significant enhancement of dielectric permittivity is needed for Al$_2$O$_3$-based materials to become suitable candidates.

Solution

To achieve the desired capacitance, we prepared composite Al$_2$O$_3$/Al thick films with different Al vol% using the aerosol deposition method [5]. Upon the application of an electric field, the free electrons of the Al particles embedded in the Al$_2$O$_3$ matrix will accumulate at the insulator/metal interfaces, acting as large electric dipoles, thereby increasing the dielectric permittivity. This is called Maxwell-Wagner polarization [6]. We successfully obtained a relative dielectric permittivity of 800 at 27 vol% Al and at 1 MHz (Figure 1a), which is a sixty-seven-fold increase compared to Al$_2$O$_3$. However, at the same time, dielectric losses, tan(δ), reached 0.58, which is much higher compared to 0.01 in Al$_2$O$_3$ thick films. In addition, a finite-element model of the composite thick films was implemented showing the similar nonlinear response of the electrical conductivity versus Al content in the composites (Figure 1b). Our results show novel possibilities for using Al$_2$O$_3$-based materials in electronic applications.
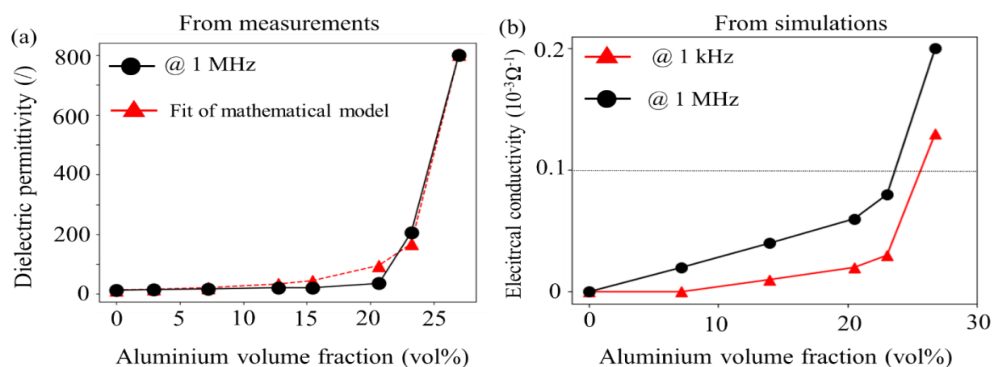

Figure 1 (a) The dielectric permittivity versus Al vol% in thick-film composites at 1 MHz and the fit of the mathematical model from percolation theory [6]. (b) Electrical conductivity at 1 kHz and 1 MHz from the finite-element simulation.

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Miniature LTCC based flow system for electrochemical detection of pesticides

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Problem

The overuse of pesticides in agriculture poses a significant risk to human health and ecosystem sustainability. Electrochemical methods provide rapid, sensitive, and inexpensive detection of compounds that can undergo a redox reaction and are widely used to detect pesticides. They can be operated with portable equipment that allows on-site monitoring [1]. The use of screen-printed electrodes (SPEs) instead of traditional bulk electrodes offers miniaturization, easier integration into portable devices, and mass production [2]. Since continuous flow conditions enhance heat and mass transfer during the reaction, resulting in increased Faradaic response, fabrication of a portable miniature flow system would not only enable continuous on-site monitoring, but also increase sensitivity and reproducibility of detection [3].

Solution

In this work, we present a miniature flow system based on low temperature co-fired ceramic (LTCC) technology with three measurement sites into which disposable SPEs can be inserted. The integrated electric heaters and temperature sensors allow temperature control, while the flow is controlled by a piston pump. The electrochemical response of commercially available SPEs (C110, Drop Sens) was measured by cyclic voltammetry (CV) in a model solution containing 5 mM $Fe(CN)_6^{3-/4-}$ as a redox probe dissolved in 0,1 M phosphate buffer solution (pH=7) at a potential of -0.6 V to $+0.8$ V. Measurements were performed at various flow rates from 0 to 5 ml/min at 25°C. At all flow rates, increased Faradaic currents were observed compared to steady-state conditions. Above 4 ml/min current plateau appears, indicating elimination of the diffusion layer at the electrode surface. CV was measured at 25 and 45°C at a flow of 4 ml/min and showed a further increase in Faradaic response. The experiments show that miniature system allows electrochemical measurements under continuous flow up to 5 ml/min and temperatures up to 50°C. It will be applied for neonicotinoid pesticide detection.

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Knee and hip joints range of movement comparison: artificial gravity vs terrestrial setting

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Problem

Exercise countermeasures (CM) are employed to mitigate the negative effects space flight poses to all physiological systems. One such CM is a short-arm human centrifuge (SAHC) with an integrated 2-axes squatting sled. It is unclear how artificial gravity affects exercise biomechanics.

Solution

12 male participants with no prior SAHC training experience completed an exercise session comprising an upright front squat in both a terrestrial setting (TS) and a squat on the SAHC (AG). Each participant completed a total of 6 sets x 6 repetitions in the following order: 1) TS before centrifugation (TSB); 2) squatting under AG; 3) TS after centrifugation (TSA). Knee and hip angles were assessed under the aforementioned conditions at 1g and 1.25g.

Knees (1g TS and AG)- the knees started the squat movement at 3.79°± 4.50°. AG reduced the range of motion (96.26°±7.28°) compared to TS (107.7°±9.39°), by 11.48°±0.38° (p=.002).
Knees (1.25g TS and AG)- the knees initiated the movement at 4.23°±5. 67°.AG reduced the ROM (95.75°±8.75°) compared to TS (110.4°±7.45°), by 15°±0.80° (p=.002).
Hips (1g TS and AG)- compared to TS, the hips began from an already flexed position (AG= 24.94°±13.63; TS= 9.88°±7.55°). Moreover, AG reduced the total ROM (65.41°±17.31°) compared to TS (114.2°±10.72°), by 49°±0.72° (p<.0001).
Hips (1.25g TS and AG)- similar to 1g, the hips began the movement from a flexed position (AG= 26.16°±13.58; TS= 8.20°±7.13°). Moreover, AG reduced the total ROM (67.86°±12.72°) compared to TS (103.2°±11.30°), by 35.24°±1.33° (p<.0001).
AG leads to a significant reduction in the knee and hip ROM during the participants' initial centrifugation. Squatting on a SAHC is not the same as a TS and further work is required to investigate adaptation to multiple SAHC sessions.

Preparation of dielectric thick films for use in fluidic thermal switches

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Problem

Vapour-compression has become a well-developed technology for refrigeration and air conditioning, however it suffers from environmental problems of refrigerants and moderate efficiency [1]. In recent years, the interest in finding alternative technologies has rapidly increased. One alternative is magnetocaloric (MC) energy conversion. Despite showing the greatest potential to replace vapour-compression in the future, today's MC devices have issues with inefficient heat transfer and hydraulic losses. In light of this, we are preparing unique fluidic thermal switches based on the electro-wetting on dielectric (EWOD) effect for MC cooling applications. With EWOD, an external electric potential can manipulate liquid droplets (e.g. change of shape, movement), which can be used to form a thermal bridge for heat transfer. Such a device consists of a multilayer structure, presented in Figure 1a. Two electrodes are needed for the EWOD effect, while dielectric layers separate the electrodes from the MC material and liquid droplet.

Solution

In this work, we prepared three different dielectric thick-film layers on gold-sputtered glass substrates and investigated their functional properties. SU-8 polymer layers were prepared using the spin-coating method while polyimide P84® NT and Al_2O_3 layers were prepared using aerosol deposition method. In the aerosol deposition, N_2 was used as the carrier gas with two flow rates: 2L/min for polyimide and 4L/min for Al_2O_3 layers. A photograph of aerosol-deposited polyimide film is shown in Figure 1b. The surface morphology and cross-sectional microstructural properties of the films were investigated using atomic force microscopy (AFM) and scanning electron microscopy, respectively. In Figure 1c, AFM topography tapping amplitude image of aerosol-deposited polyimide thick film on a glass substrate is shown. The root-mean-square roughness of these films measured with contact profilometry is $R_q \sim 800$ nm. In this contribution, the dielectric properties of prepared ceramic and polymer thick-film layers will also be discussed.
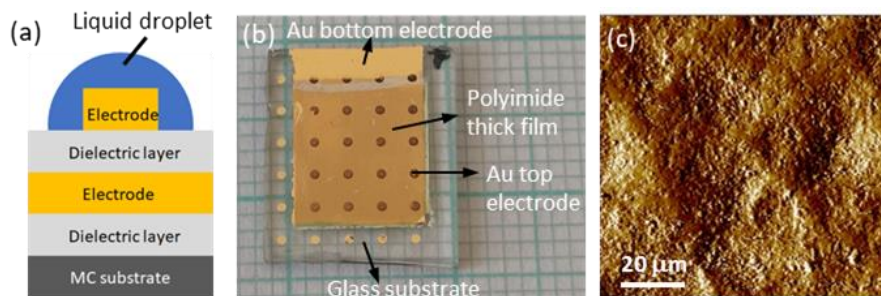

Figure 1: (a) Schematic presentation of multilayer structure. (b) Photograph and (c) AFM topography – tapping mode amplitude image of polyimide thick film on glass substrate prepared by aerosol deposition technique.

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Inactivation of viruses in water via low-pressure plasma irradiation

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Problem:

Some viruses can cause severe health problems, requiring their removal from any materials and mediums we interact with. Water serves as a transmission medium, enabling viruses to spread to their host, causing an infection. Inactivating viruses in water usually entails using chemical disinfectants, filtration techniques, oxidants, or UV radiation, which can be environmentally problematic, difficult to maintain or inefficient. Low-pressure plasma radiation is a unique source of highly energetic vacuum ultra-violet (VUV) photons that can disrupt the viral structure, resulting in viral inactivation, while also producing highly oxidative compounds, such as OH radicals, which provide additional antiviral activity. However, it is difficult to generate low-pressure plasma in the presence of liquid water. Additionally, VUV radiation is completely absorbed by oxygen in the air, precluding the application of ultra-violet radiation to liquid samples.

Solution:

To treat water with a low-pressure plasma, we have constructed a hermetically sealed chamber with an MgF_2 window facing the plasma source. Within this chamber we enclosed a water solution of MS2 bacteriophage in a nitrogen atmosphere, allowing the VUV radiation to reach the sample. The solution was treated with low-pressure (500 Pa) H_2 plasma radiation, ignited with a DC-pulsed generator at 50W. Plasma radiation alone was sufficient to inactivate 99% of viruses within 5 minutes of treatment, and after 10 minutes no viruses were detected in the sample. The reaction between OH radicals and terephthalic acid produces hydroxyterephthalate (Figure 1), confirming the generation of OH radicals, which may be responsible for the observed viral inactivation.
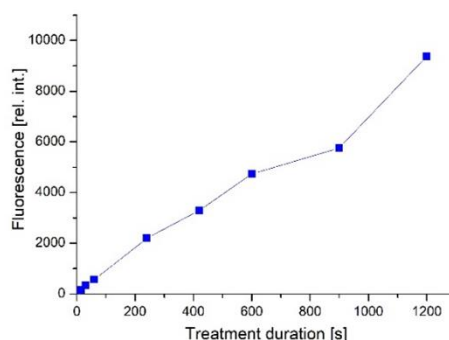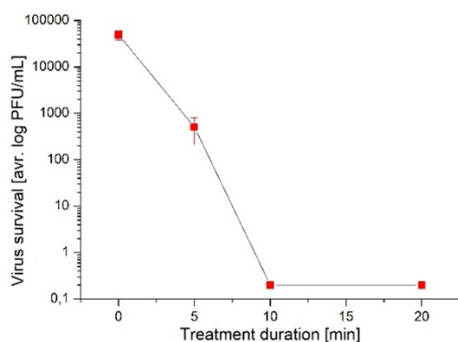
Energy storage properties of (1–x)Pb(Fe0.5Nb0.5)O3–xBiFeO3 bulk ceramics and thick films

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Problem

Energy storage is the ability to collect and store energy for use at another time. Dielectric capacitors have higher power density compared to batteries and are good candidates for energy storage 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]. Such properties are obtained in $(1-x)\text{Pb}(\text{Fe}_{0.5}\text{Nb}_{0.5})\text{O}_3-x\text{BiFeO}_3$ (PFN–100xBFO) solid solutions. Compared to bulk ceramics, thin films withstand higher electric fields, which makes them even more promising for energy storage applications [2].

Solution

In this work, we investigated the energy storage properties of PFN–100xBFO bulk ceramics and thick films. PFN–100xBFO (x = 0–0.5) powders were prepared by mechanochemical synthesis. The isostatically pressed pellets were sintered in an oxygen atmosphere at 950 °C (x = 0–0.1) and at 900 °C (x = 0.2–0.5) for 2 h. The recoverable energy storage density (U_{rec}) and efficiency (η) were calculated for all compositions (Fig. 1a). The best properties were determined for the composition x = 0.3, which exhibits slim and pinched P–E hysteresis loop (Fig. 1b). The U_{rec} and η values at 70 kV·cm^{-1} are 0.9 J·cm^{-3} and 82%, respectively. Furthermore, PFN–30BFO films were prepared by screen-printing the thick-film paste on $\text{Au}/\text{PbZr}_{0.53}\text{Ti}_{0.47}\text{O}_3/\text{Al}_2\text{O}_3$ substrates. The samples were sintered in an oxygen atmosphere at 800 °C for 2 h. The U_{rec} value of the sample is 2.2 J·cm^{-3} at 350 kV·cm^{-1}, which is higher compared to the U_{rec} value of the bulk ceramic due to the higher electric field. On the other hand, the η value for the thick film at 350 kV·cm^{-1} is 54%, which is lower than that of the bulk ceramic due to the wider P–E hysteresis loop (Fig. 1c).
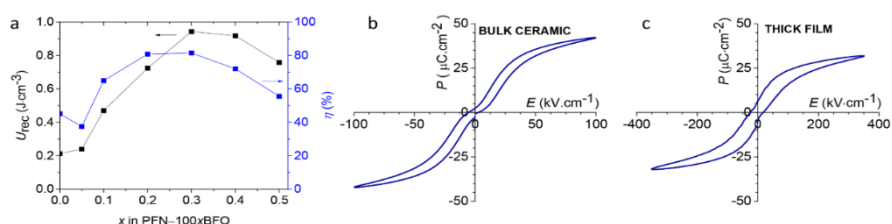

Figure 1. (a) The U_{rec} and η at 70 *kV·cm^{-1}* versus PFN–100xBFO bulk ceramic compositions. *P*–*E* hysteresis loop for (b) PFN–30BFO bulk ceramic (after [3]) and (c) screen-printed PFN–30BFO thick film. Note the differences in the scales of *E*.

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