1st – 3rd June 2022, Kamnik, Slovenia

Jožef Stefan Institute

Better communication science

BOOK OF ABSTRACTS

14th Jožef Stefan International Postgraduate School Students' Conference

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14. ŠTUDENTSKA KONFERENCA MEDNARODNE PODIPLOMSKE ŠOLE JOŽEFA STEFANA

Knjiga povzetkov

14th JOŽEF STEFAN INTERNATIONAL POSTGRADUATE SCHOOL STUDENTS' CONFERENCE

Book of abstracts

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IPS student council (eng)

So here we are. After two years of self-isolating, mask wearing, social distancing, and having a cotton-covered stick jammed into our nasal cavities regularly, it seems like we are (finally) getting to a place where everyday life seems familiar and, dare I say, normal. Gone are the days when we would listen to the news, hopeful, that the infections are down and that restrictions would soon follow. Now the new infection rates are hardly mentioned, and the rapid tests are slowly gathering dust in the cupboards. Yes, things are looking up, but we remain cautious, as we've been in a similar situation last year. With the wide administration of vaccines, immunization, and milder variants, hopeful we remain, that the pandemic period will not exceed the year 2022 in the history books. Sadly, with the current situation developing in Ukraine, we are reminded that we should not become complacent in striving to rid the world of terrible tragedies, and that only together we can make life safe and prosperous for all.

We are pleased to say that the 14th International postgraduate student conference (IPSSC) will be held in person. Close to 100 students, faculty members and company representatives will gather in Kamnik, at the Mekinje monastery. There they will showcase their research, debate different perspectives and share their ideas, surrounded by picturesque mountains and plains of Kamniško-Savinjske Alpe. The title of the event is "better communication – better science", which the organisers chose because of its demonstrated relevance in the current environment of false claims and misinformation. Students are fully aware that effective communication is crucial to demonstrate one's discoveries, present facts and engage your listeners. Great science is often overlooked due to poor communication, therefore invited speakers and lecturers will give their insights on how to succeed in a world overflowing with information and noise. We are also pleased to say that this year we have an abundance of institutional and corporate support, realising the importance of this event and doing their part in developing young researchers to develop themselves and their careers.

The conference organizing committee has been working tirelessly throughout the year to make sure that participants feel welcome, appreciated, and enthusiastic to network with their colleagues. The students, with the help of IPS professors and mentors, have once again provided an excellent line-up of abstracts, posters, and presentations, which will be at the centre of daily proceedings, and will no doubt spark a lot of discussions thereafter. For some of them this will be the first time when they are able to meet face-to-face with their fellow classmates and that is something to be excited for. We would once again like to thank the IPS and IJS professors and faculty members, our sponsors and our great organising committee for making all of this possible. And with that, the lights are off, the curtains are raised, and the crowd is in their seats.

Let the show begin!

The IPS Student Council

Beseda predsednika MPŠ: Akad. prof. dr. Vito Turk (slo)

Zadnji dve leti smo živeli in delali v pogojih, ki jih v moderni dobi človeštvo še ni poznalo. To je bila posledica pandemije, ki jo je povzročil koronavirus (Covid-19) in prizadel vse kontinente in države, tudi Slovenijo. Hitro smo se morali prilagoditi novemu načinu vsakodnevnega življenja, kar je terjalo veliko samodiscipline ter odgovornosti na vseh ravneh. Šele pred kratkim se je širjenje tega nevarnega virusa upočasnilo in končno vsaj začasno skoraj ustavilo, tako, da smo lahko zopet vsaj približno normalno zaživeli.

Tudi naša Mednarodna podiplomska šola Jožefa Stefana - MPŠ se ni mogla izogniti posledicam pandemije. Vse naše aktivnosti smo bili prisiljeni prilagoditi novim razmeram, kar je terjalo tako od vodstva šole, profesorjev in mentorjev , drugih sodelavcev in seveda naših podiplomcev popolnoma nov pristop k reševanju nastale situacije. Ob tem pa se je pokazalo, kako ključnega pomena je dobra organiziranost in sodelovanje na vseh ravneh delovanja podiplomske šole. Tudi delo v raziskovalnih laboratorijih je potekalo uspešno ob upoštevanju vseh predpisanih zaščitnih pogojev. Prepričan sem, da smo se v tem pogledu najbolje odrezali v Sloveniji, za kar gre vsem sodelujočim izjemna zahvala!

MPŠ deluje že skoraj 20 let in je v tem času svojo ustanovitev več kot potrdila s svojim kvalitetnim delovanjem. Danes je MPŠ doma in v mednarodnem prostoru uveljavljena podiplomska institucija. Seveda pa tega ne bi bilo brez vpetosti uglednih raziskovalnih institutov v delovanje šole. Na prvem mestu naj omenim Institut Jožef Stefan, ki največ doprinaša k uspešnemu delu te šole z odlično opremo vključno s Centri odličnosti, sodobnim znanjem in kvalitetnimi mentorji. Prav tako je pomembna vključitev Nacionalnega inštituta za biologijo – NIB in Inštituta za kovinske materiale in tehnologije - IMT v delovanje šole. Vse to pa kaže na interdisciplinarno naravnanost, ki je ključnega pomena za razumevanje sedanjega časa, ob inovativnosti in odličnosti. Pojem “odličnost” se je v svetu uveljavila, še zlasti na področju znanosti. Ni dovolj, da se tega zavedamo raziskovalci, pač pa to morajo razumeti tako politiki, ki vodijo državo, in gospodarstvo. Da so naši doktorandi uspešni, dokazujejo številne odlične publikacije in podeljeni patenti, kar našo MPŠ uvršča glede na njeno velikost v sam vrh slovenske znanosti ! Rezultati osnovnih raziskav in osvojenih novih znanj vodijo s svojimi prelomnimi dosežki do novih inovacij in proizvodov z visoko dodano vrednostjo, ter krepko višjim BDP, od katerih je odvisna ekonomska rast in moč države, tudi Slovenije. Zato pa je potrebno veliko naporov in finančnih vlaganj vlad, ki razumejo pomen znanosti in raziskav za razvoj celotne družbe. To velja še zlasti v današnjem kriznem obdobju. Izhod iz tega nam bo omogočilo le znanje ! To dokazujejo uspehi razvitih držav, ki ves čas povečujejo vlaganja v znanost in razvoj, dodatno pa so še povečali v času pandemije. V Sloveniji pa nasprotno stagniramo že vsaj 10 let kljub nenehnim obljubam o povečanju vladnih vlaganj v raziskave in razvoj na 1% BDP. Trenutno so vladna vlaganja v ta resor med 0.3-0.4 % BDP , kar nas uvršča na dno EU. Upamo, da bo nova vlada bolje razumela pomen znanosti, ki bo omogočil priključitev Slovenije med razvite države Evropske

skupnosti do leta 2030! Tako bi tudi zaustavili beg možganov, ki je ta čas največji, kar smo jim priča pri nas!

Tudi letošnja predstavitev raziskovalnih dosežkov naših podiplomcev, je ponoven dokaz njihove uspešnosti. To vam omogoča, da se boste ob pomoči mentorjev ter vseh sodelujočih razvili v kreativne raziskovalce, na katere bomo ponosni. S svojem znanjem boste doprinašali k boljši prihodnosti, kot vam jo ponuja sedanjost. Vso pravico imate, da se uspešno spopadate z izzivi v domačem okolju, ne pa da iščete izpolnitve svojih ambicij in eksistenčnih možnosti z odhodi v tujino, pogosto brez povratka.

Ob koncu, bi še enkrat ponovil in kar sem že večkrat izjavil: “Znanje je vrednota, ki omogoča narodu ekonomski razvoj in obstoj. Osnovne raziskave sodijo v ospredje moderne kulture in nam pomagajo razumeti, kdo smo “! Mladi vrhunski raziskovalci so pogoj za uspešen gospodarski in vsesplošen razvoj. So srce družbe znanja. Očitno so potrebne za to spoznanje globoke družbene spremembe, katerih pa do sedaj še nismo dočakali. Vendar bodimo to pot optimisti, saj upanje umre zadnje!

IPS Dean's words, Prof. Dr. Milena Horvat (eng)

The time of the pandemic and the restriction of social interactions is history, therefore IPS students enthusiastically decided to hold the traditional annual conference in person. It is therefore no surprise that "Better communication – better science« is also a central theme of this year's conference. Undoubtedly, in the essence of every student, there is a clear awareness that communication can only be effective if excellence, creativity and innovation are behind the results of scientific work. In order to communicate effectively, in addition to modern social approaches, it is necessary to ensure social contacts – this is the only way to achieve effective and significant progress in the cooperation within and between different scientific disciplines of the IPS study programme and wider, including various 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 the 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 programmes 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 the IPS conference demanding organisational task was entirely in the hands of the Organising Committee and the IPS Student Council. IPS and its partners are extremely proud of their commitment and excellent organisation. 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, their 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, support staff, partners and founders of the school.

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

Povzetki / Abstracts

Ekotehnologija (Ecotechnologies)

Application of multi-elemental and Sr isotopes analysis in provenance of dairy production in Naxos, Greece

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The milk and dairy products authenticity has frequently been verified by means of stable isotope analysis of light elements. Recently, however, non-traditional isotopes, such as Sr isotopes, have proven to be promising geographical tracers [1]. It has been found that $^{87}Sr/^{86}Sr$ is not modified during the uptake of the plant and it is transferred unchanged to all living organisms in the food chain, which enables tracing trends in the soil-vegetation system [2]. The present study is aiming at verifying the ability of multi-elemental and Sr isotopic fingerprint to differentiate the origin of milk and cheese samples from different areas of Naxos, Greece, by linking milk and cheese data with those corresponding to soil, water and forage from the same production areas. Naxos is the largest Cycladic island located in the center of the Aegean Sea in Greece. Geology settings of the island, mountainous terrain, hydrographic network and abrupt changes in topography observed between different lithological formations reflect the inorganic pattern of a food commodity. Being home to widely-recognized PDO cheeses, the island is an important part of global isotopic composition database. For the study purpose, multi-elemental composition and Sr isotope ratio were determined in samples of different types of milk and cheese, water, soil and feed. Samples were collected at different farms, during summer and winter season, through two years of production. The contribution of Sr isotope ratio from water and feed in the milk and cheese Sr isotope ratio will be evaluated, which would allow a more accurate characterization of the milk and cheese provenance and provide an integrated overview on links between studied matrices and areas. The elemental composition of the samples was determined by inductively coupled mass spectrometry (ICP-MS) after microwave digestion of samples, while Sr isotope ratio was determined by multi-collector ICP-MS, after performing Sr isolation from the matrix procedure.

References:

[1] S. Hamzić Gregorčič et al., *Foods*, 2021, *10*, 1729.
[2] J. Griboff et al., *Food Chemistry*, 2019, *283*, 549-558.

Associations of ALAD gene single nucleotide polymorphisms with blood lead concentrations in pregnant women

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A lot of research conducted in the last decades points to individual genetic variances playing a role in susceptibility and adaptability to metal(loid)s toxicity. Delta-aminolevulinic acid dehydratase (ALAD) gene polymorphisms present one of the genetic polymorphisms heavily studied in relation to blood-lead (B-Pb) concentrations and Pb toxicity. However, research conducted on pregnant women is scarce, and results at low exposure levels are inconclusive. Therefore, our aim was to assess the influence of four *ALAD* single nucleotide polymorphisms (SNPs) (rs1800435, rs1805313, rs1139488, and rs818708) on B-Pb concentrations in a population of Italian pregnant women aged 17 to 44 years old exposed to low levels of Pb participating within the PHIME study. For pregnant women, Pb is especially challenging as it can be triggered to be released from the bone during pregnancy, presumably increasing B-Pb concentrations. Therefore, B-Pb concentrations reflect not only current exposure but previous as well, such as exposure to leaded gasoline, banned in Italy in 2002.

Women's peripheral venous blood samples (n=873) were collected in their 2nd or 3rd trimester and analysed for selected trace elements with Coupled Plasma Mass Spectrometry (ICP-MS) and used for DNA extraction. SNPs genotyping was performed by q-PCR using predesigned TaqMan SNP Genotyping Assays. Multiple linear regression models (STATA12/SE) were used to examine the associations between ALAD SNPs and B-Pb concentrations while controlling for mother's age, pre-pregnancy BMI, parity, education, estimated gestation week of pregnancy at blood sampling, seafood intake frequency, smoking, blood zinc concentrations, and new-born sex.

The geometric mean of B-Pb was 11 ng/g (range: 3-60 ng/g, median: 11 ng/g), which indicates a low exposure level. Three *ALAD* SNPs showed an impact on B-Pb concentrations, namely rs1800435, rs1805313, rs1139488, whereas for *ALAD* SNP rs818708 no associations with B-Pb concentrations were found. Carriers of the minor allele for *ALAD* SNP rs1800435 showed 9% lower B-Pb concentrations in comparison to non-carriers (p=0.024). Similarly, *ALAD* SNP rs1805313 homozygous carriers of the minor allele had 11% lower concentrations of B-Pb than homozygous carriers of the common allele (p=0.031), whereas homozygous carriers of the minor allele for *ALAD* SNP rs1139488 had 13% higher B-Pb concentrations in comparison to homozygous carriers of the common allele (p = 0.030).

Within our study, associations between three *ALAD* SNPs (rs1800435, rs1805313, and rs1139488) and B-Pb concentrations were found and confirmed with linear regression models in Italian pregnant women with low Pb exposure.

Cadmium exposure in Slovenian population of children and adolescents and genetic susceptibility

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Within the national Human biomonitoring programme, exposure to Cd was assessed in the population group pf children and adolescents residing in potentially contaminated areas of Slovenia. Exposure to Cd in these areas can occur through drinking water and food grown in contaminated soil. Besides industrial activities, use of phosphorous fertilizers in agriculture can contribute to elevated levels of Cd in soil. We measured Cd levels in three different biological matrices of 1099 participants aged 6-9 and 12-15 years old. As an analytical detector for measurements of Cd concentrations inductively coupled plasma mass spectrometer with three quadrupoles was used and the data about the individual's lifestyle, living environment and dietary habits were obtained by carefully constructed questionnaires. Associations between Cd levels in blood, urine and hair samples of participants, and different determinants of Cd exposure were explored using descriptive statistics, non-parametric Kruskall-Wallis's test as well as parametric tests (one-way ANOVA and Pearson's correlation).

Environmental data used for evaluation of Cd exposure within this research have shown that the levels of Cd in soil are the highest in the area around Jesenice region and the lowest around Prekmurje area, which reflects very well in the levels of Cd measured in the biological samples of participants. The highest levels of blood Cd and urine Cd were detected in Jesenice and the lowest in Prekmurje region ($p<0.001$). The highest hair Cd levels were recorded in participants residing in Mežica Valley and the lowest again, in the population part of Prekmurje region ($p<0.001$). In contrary to blood and urine Cd levels ($p<0.001$ for both), results for Cd in hair were higher in children than in adolescents ($p<0.001$). We detected no differences among sexes in blood or urine Cd levels. However, higher levels of Cd in hair were measured in boys than in girls ($p<0.001$). Comparing the exposure data with previous studies in children from Slovenia, no significant trend in levels was observed for the last decade. Overall, the levels were higher in rural over urban areas and the highest in industrial areas in the present study.

In addition, an association of Cd levels in the studied population with the gene polymorphism of individuals was done. We analyzed a SNP (=Single Nucleotide Polymorphism); metallothionein - MT2A, which was selected according to the literature and is believed to play a role in the mechanisms of cadmium uptake, metabolism and excretion. MT2A rs28366003 was genotyped in 737 study participants, and we discovered that only 9 % of the studied population carries the less prevalent genotype which can be responsible for making humans more susceptible to the absorption of Cd in their body. Overall, no statistically significant difference in blood or urine Cd levels was observed between carriers of the variant allele and carriers of the common allele. Nevertheless, geometric mean of blood Cd levels among the variant allele carriers was higher in girls (0.15 µg/L) than in boys (0.13 µg/L).

Chemical sensitivity of MeV-SIMS imaging mass spectrometry

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MeV-SIMS is a novel promising technique for chemical imaging of biomolecules in organic tissues. Known as Secondary Ion Mass Spectrometry excited by primary ions in MeV energy range, it excites electrons within bombarded matter, which leads to desorption of high-mass molecules from the sample surface. Such desorption, which is caused by primary ions losing energy through electronic excitations, instead of nuclear collisions, leads to less fragmentation of complex biomolecules.
In combination with the Time-of-Flight mass spectrometer, spectra comprise a broad mass range and simultaneous detection of desorbed ions, providing the chemical structure information, where the intensities of that ions are dependent on m/z (mass-to-charge ratio) values. Ionization of the surface organic molecules in the form of protonation or cationization with attached hydrogen or alkali metals to the molecule gives a result in significant variations of the secondary ion yield, which is defined as a number of secondary ions per primary ion. Dependence of ionization probability on the matrix, surrounding the sample, was studied with polyethylene glycol, which was mixed with various concentrations of salts, containing alkali metals Na and K. Addition of such salts lead to increase of the ionization probability by more than one order of magnitude **when even small amounts of Potassium or Sodium were mixed into the matrix.**

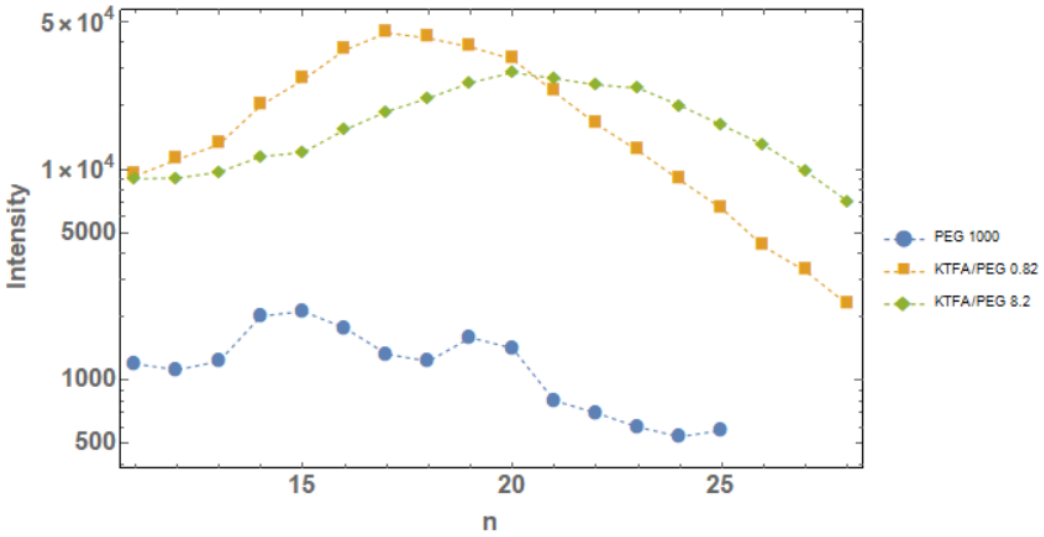

Figure 1. Intensity of $[M_n+K]^+$ peaks for various concentration ratios. Lines are drawn to guide the eye. With increased amount of added KTFA, the centre of peak intensities moves to higher n.

Acknowledgments:

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Discrimination of Slovenian pork meat according to geographical origin

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Proof of provenance has increased in relevance over the past decade because of its positive impact on food safety, quality and consumer protection. This trend has created interest in building local and regional food systems across Europe, including Slovenia. This study will present how we can verify that pork meat on the Slovenian market corresponds to its declaration using isotopic and elemental analysis, one of the most powerful approaches for determining geographical origin [1,2]. In order to evaluate the authenticity of commercial food samples, the isotopic and elemental data must be compared with reference data from a databank of authentic samples and evaluated in terms of their match within statistical limits. For the databank, 70 Slovenian pork meat samples were collected from farms in four different regions, while the correct labelling has been verified on 18 commercial samples labelled as Slovenian obtained from different Slovenian grocery stores. In all samples, the isotopic composition of light elements (δ13C, δ15N and δ34S) was determined by IsoPrime100 – Vario PYRO Cube Isotope Ratio Mass Spectrometer (IRMS). The isotopic composition of oxygen in isolated water from the meat was determined by an IsoPrime MultiFlow system coupled to IRMS. The elemental content in pork was measured by inductively coupled plasma mass spectrometry (ICP-MS). We anticipate that the outcomes of this research will be helpful for government agencies to verify the origin of pork meat, for consumers who wish to be protected from food frauds, and farmers who would like to protect their Slovenian pork meat.

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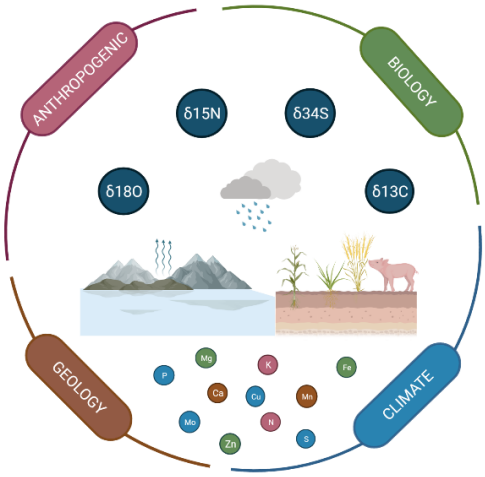

Figure 1. Graphical abstract

Distillation as Isolation Method for the Determination of Methyl Mercury Compounds in Urine Samples

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Mercury is a highly toxic naturally-occurring heavy metal that is a well-known threat to human health and the environment. Several forms of mercury are present in the environment: elemental, inorganic and organic mercury. Each of these forms has a unique toxicological profile, mechanism of transport and deposition in the body and different metabolic fate. With regards to human exposure and adverse health effects, the most important form of mercury is methylmercury (MeHg), to which humans are exposed through diet, predominantly through fish consumption. In order to well understand mercury's toxicity, in addition to total amount, also the amount of existing species in different biological matrices should be determined. Speciation analysis has become an essential prerequisite for conducting reliable and reasonable risk assessment. In the present study, speciation of urine samples was performed and feasibility of distillation as isolation method was investigated. First, MeHg compounds were isolated from urine samples by distillation, after which followed aqueous phase ethylation, precollection on Tenax trap, isothermal gas chromatography, pyrolysis and cold vapour atomic fluorescence spectrometry detection (CVAFS). Additionally, results obtained with distillation as the isolation method were compared with results obtained with acid digestion (4M HNO_3) instead of distillation. Good agreement between the results was found in samples with MeHg concentration above 2 pg g^{-1} urine, which was the limit of detection when using acid digestion for isolation of MeHg compounds. On the other hand, using distillation as the isolation method led to a lower limit of detection of 1 pg g^{-1} urine. Moreover, distillation provided high and consistent recoveries (91±4%) and more accurate results at low MeHg concentrations. It also provides significant savings in sample preparation time compared to acid digestion (few hours vs. few days) and enables avoidance of matrix interferences, that are the most important limitation of acid digestion when determining low MeHg levels. Additionally, a case study was conducted, in which 6 volunteers (3 females and 3 males) consumed 300 grams of tuna steak after which MeHg concentrations in blood and urine were followed over the period of 1 month. The goal is to gain first insight in urinary excretion patterns of MeHg, which, to our knowledge, has not been so far.

Do you trust your measurement? Atmospheric mercury (Hg) case study

Jan Gačnik [1,2], Igor Živković [1], Sreekanth Vijayakumaran Nair [1,2], Teodor-Daniel Andron [1,2], Jože Kotnik [1,2] and Milena Horvat [1,2*]

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The abundance of available and emerging analytical methods in the field of environmental science, although beneficial to the field, has led to increased requirements for proving the validity of the measurement result. The results obtained by different analytical methods with different calibrations can only be compared with each other with a statement of traceability and uncertainty for the measurement result. Neglecting the traceability and uncertainty of the measurement result is also one of the key factors hindering comparable atmospheric mercury (Hg) speciation measurements. Atmospheric Hg speciation concerns three main Hg species: gaseous elemental (Hg^0, GEM), gaseous oxidized (Hg^{II}, GOM) and particulate-bound (Hg-p, PBM) mercury. All of these species face a variety of analytical challenges connected to their chemical/physical properties and low ambient concentrations. GOM and PBM are more reactive and less abundant than GEM and as such face the majority of the analytical problems. Our work focused on GOM analytical methodology, specifically on GOM sampling and calibration. Different GOM sampling methods (sorbent traps, denuders and cation-exchange membranes) and calibrations (evaporative calibrators and permeation-based calibrators) were compared, with emphasis on the use of ambient concentration levels. Additionally, we developed and validated a novel GOM calibration method based on non-thermal plasma oxidation of elemental mercury. All investigated analytical methodology was evaluated in terms of feasibility for the intended use, measurement uncertainty and traceability. ^{197}Hg radiotracer was used for validation of the aforementioned analytical infrastructure due to its high sensitivity and selectivity, which enabled ambient level concentration experiments.

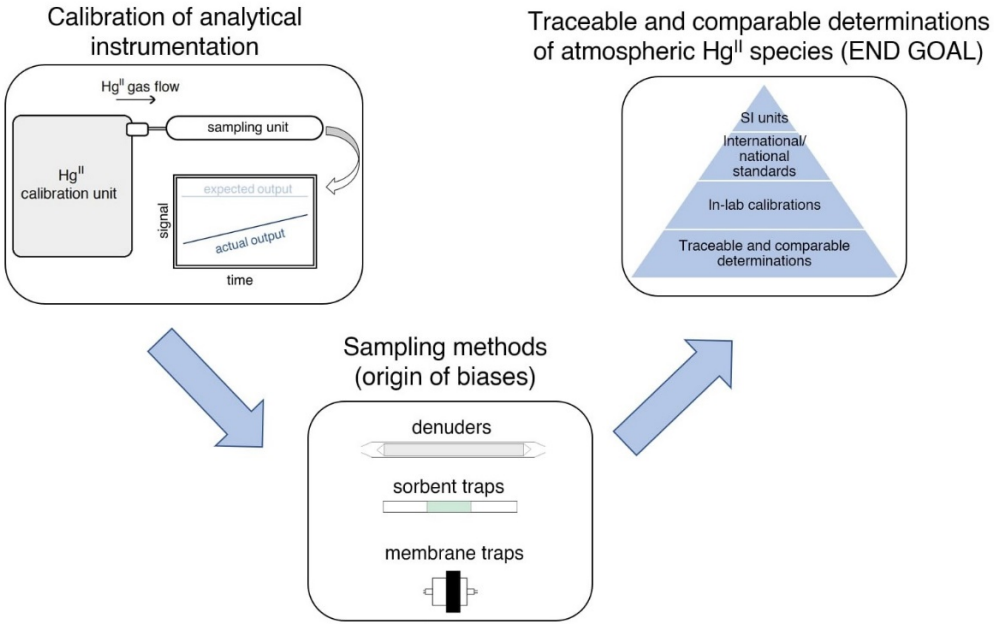

Figure 1. Gaseous oxidized mercury (Hg^{II}, GOM) calibration and sampling methods: aim for improvement and establishment of traceable Hg^{II} measurements.

Effects of Treated Wastewater Irrigation on Tomato Fruit Quality Attributes

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Tomatoes are a popular fruit consumed worldwide, both fresh and processed, and are considered a good source of minerals and vitamins, proteins, essential amino acids, monosaturated fatty acids, carotenoids, and phytosterols. They grow readily in warm climates and colder climates under glass; however, they require substantial irrigation. Slovenia is an alpine country considered rich in freshwater resources; however, regions of the country, for example, Vipava valley and the coast face a shortage of drinking water in the summertime. Regarding the circular economy, irrigation with treated wastewater could reduce river and groundwater extraction in areas subject to water stress. The problem is that, although treated municipal wastewater is a source of nutrients, it also potentially contains pollutants, and when applying treated wastewater for irrigation, its effect on the safety and quality of the fruit needs to be assessed. Our study aimed to assess the effects on fruit quality by comparing tomatoes irrigated with potable water and treated wastewater. For this purpose, we grew tomato plants in soil and hydroponically. In the case of soil-grown tomatoes, they were grown in lysimeters and were irrigated with: a) potable water with commercial fertilizer, b) wastewater effluent, c) wastewater effluent spiked with 14 model contaminants of emerging concern (CEC) (0.1 mg L^{-1}). In the case of hydroponically produced tomatoes, the plants were irrigated with: a) potable water with fertilizer b) potable water with fertilizer spiked with CEC (0.1 mg L^{-1}). The model CEC included industrial chemicals (bisphenols), pharmaceuticals (non-steroidal anti-inflammatory drugs, estrogens), and common stimulants (caffeine). The quality of the tomato fruits was assessed in terms of the amino acids, lipids, aroma profile, and elemental composition using optimized and validated methods based on HS-SPME GC-MS, LC-MS/MS, and ICP-MS. These quality parameters were chosen since they influence flavor, texture, structure, mouthfeel, the color of tomatoes, and the content of bioactive compounds and specific elements that promote good health. The preliminary results of our study will be presented.

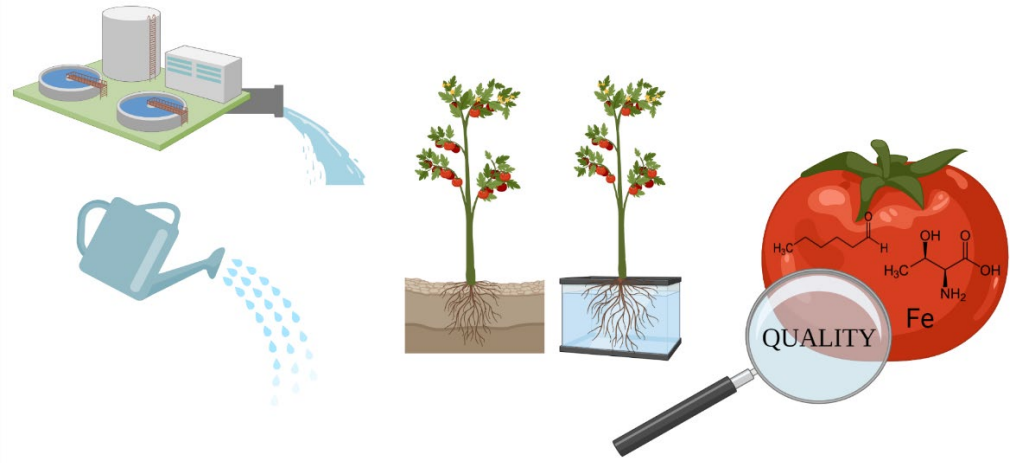

Figure 1 Tomatoes grown in soil and hydroponically, irrigated with wastewater and potable water

Elemental and Pb Isotope Composition in Water and Sediments from the Meža River Catchment

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The upper Meža Valley has centuries long history of both mining and smelting of Pb and Zn ores. During processing, a large amount of mine waste, which contained high concentrations of Pb, Zn, As, Cd and other potentially toxic elements (PTE), was produced and deposited in abandoned mine shafts and near small streams at more than 30 locations along the upper Meža Valley. As a consequence, the Meža river and its tributaries were highly contaminated with Pb and other PTE [1]. But as mine tailings began to be deposited in abandoned parts of the mine and as water treatment plants were constructed, the concentrations of Pb and other PTE in the water began to decline [2]. However, the concentrations still remained high in sediments, ranging from 100 to 19,000 mg/kg [1,3]. Some other industries were also established in the area during the last few decades.

Although the concentrations of PTE and especially of Pb in the Meža river decreased over time, they still persist in quite elevated levels. At present there are no data on the isotope composition of Pb in the water and sediment samples taken from the area. Therefore, the objectives of the present study were i) to determine the concentrations of PTE in the water and in the two fractions (<0.063 mm and <0.150 mm) of sediment samples from the Meža river and its tributaries, ii) to compare the results with previous studies and see if the PTE concentrations decreased or increased as time passed, iii) to determine the Pb isotope composition in the water and sediment samples from the upper Meža Valley, and iv) on the basis of a Pb isotope fingerprint, determine its sources in sediment and water samples.

For the analysis, sediment samples were digested with a closed vessel microwave assisted digestion. Total elemental concentrations were determined by quadrupole ICP-MS and the Pb isotope ratios were determined by MC ICP-MS, coupled to a desolvation system.

The results showed elevated Pb and Zn concentrations in water and sediments at the majority of sampling sites. The highest measured average concentrations in water were of Zn, followed by Pb, As and Cd. The average Pb concentrations determined in this study were higher than the threshold values set by the EU Water Frame Directive (WFD) (7.2 µg/L) [4]. The limits were exceeded at the majority of sampling sites. In general, higher concentrations of Pb, Cd and As were determined in sediment fraction <0.063 mm, while Zn was higher in <0.150 mm fraction. The isotope composition of Pb in both fractions and between different sampling locations slightly differed, indicating an additional Pb source.

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Evaluation of probiotic potential of bacteria isolated from human oral samples

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Two of the most common bacterial diseases of man are periodontal disease and caries that develop in the habitat of the oral cavity as a result of imbalance of the oral microbiome and activity of the host immune system [1]. Healthy oral microbiome consists of pathobionts and commensal microorganisms that are interacting with the host. Accordingly, one of the theories describing the development of the periodontal disease proposes that there is a particular microbiome-host interaction that leads to the overgrowth of the pathobionts resulting in the disease [2]. Therefore, based on this assumption we hypothesized that among the oral microbiome of healthy individuals there must be probiotic species that prevent the progression of inflammation.

The aim of the research is to isolate bacterial strains from human oral samples and test for their potential antimicrobial effect against the well-known pathobionts involved in the disease such as *Aggregatibacter actinomycetemcomitans, Fusobacterium nucleatum* and *Poprhyromonas gingivalis*. However, as there are no recommended MIC determination methods for anaerobic bacteria, different antimicrobial assays had to be tested. Here we developed an antimicrobial assay to select for potential probiotic strains acting against anaerobic strains. The assay will be used for screening for potential antimicrobial activity of isolated strains. Strains that will show antimicrobial activity against pathogens will be characterized and 16S rRNA gene based phylogenetic analysis will be used.

The preliminary results show that 150 isolated strains express antimicrobial effect against *E. coli* and these selected strains will be tested against anaerobic pathobionts. Strains that will exert antimicrobial activity will therefore be considered as probiotic candidates and further evaluated for potential use as oral therapeutics. In light of prevalence of oral diseases on the one side as well as antibiotic resistance on the other, the advantages of the probiotic therapy lie in the ability to prevent and ameliorate microbiome imbalance through microbial interactions.

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Food and feeding habits of *Serranus scriba*, an important mesopredator in the northern Adriatic Sea

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Serranus scriba (Linnaeus, 1758) is a common member of coastal fish assemblages in the northern Adriatic Sea, which inhabit nearshore rocky habitats and seagrass meadows. For the diet analysis, non-lethal and non-destructive method based on fecal pellet examination was used. Analysis of prey remains in faecal pellets confirmed that *S. scriba* preys on decapods, polychaetes, isopods, molluscs, swarming shrimps, and fish. Anomurans (especially *Pisidia sp.)* were the main prey of *S. scriba* in the northern Adriatic. The study also confirmed that older and larger individuals prey on larger prey, while smaller individuals prefer smaller, but more numerous prey. This change in feeding habits and predatory behaviour is referred to as an ontogenetic shift. The calculated index of trophic diversity (ITD) of 0.89 indicates that *S. scriba* is an opportunist that feeds on a wide range of different prey. The calculated trophic level of 3.43, which is higher than that of other members of the community, is indicating that S. scriba is also an important piscivorous predator. In addition, trophic level increased with age. The proportion of crustaceans, gastropods, and polychaetes in the diet decreased with age and body size, while the proportion of fish increased. Prey composition depended also on the bottom type where *S. scriba* was captured. Due to its opportunistic feeding behaviour, the diet of S. scriba directly reflects changes in the environment, and is therefore suitable as a bioindicator species for the implementation of Descriptor 1 of the Marine Strategy Framework Directive.

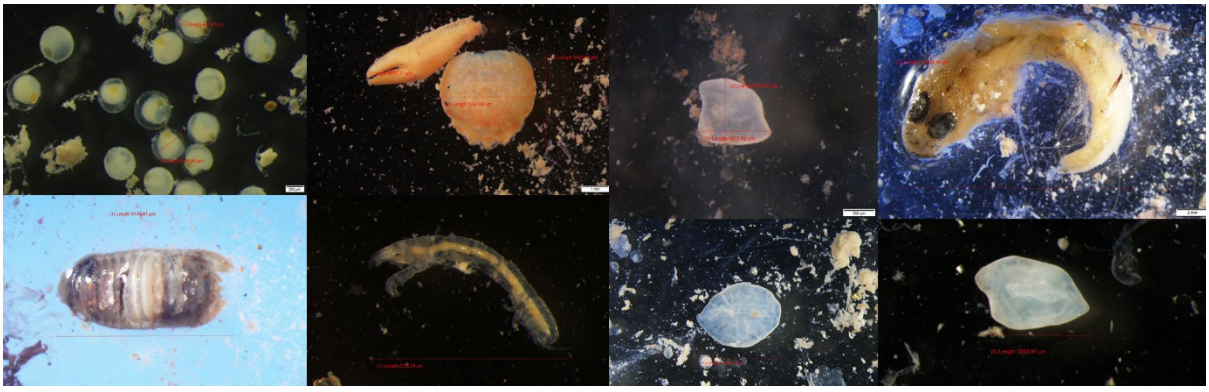

Figure 1.: Prey items found in fecal pellets of *S. scriba* (in clockwise direction: fish eggs, claws and carapace of Pisidia sp., otolith of *Gobius fallax*, undigested *Gobius sp*., isopod - family Sphaeromatidae, *Tanais dulongii*, otolith of *Atherina hepsetus*, otolith of *G. cruentatus*).

Acknowledgments:

The authors would like to thank Milijan Šiško, Tihomir Makovec, Leon Lojze Zamuda, Luka Preložnik, Jure Zaman, Urška Bizjak, Gaja Jenko, Mojca Pungerčar, Doroteja Erhatič and Romina Bonaca for their assistance during the fieldwork and laboratory work. Special thanks to dr. Valentina Pitacco and Milijan Šiško for their help in the statistical analyses.

FoodTrack – stable isotope tool for determination of authenticity and investigating food fraud

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Background

Consumers are becoming ever more aware of food fraud and are increasingly interested in knowing the provenance and authenticity of their food. Methods for food authenticity testing require robust analytical techniques that play an essential role in creating trust and ensuring food quality and traceability throughout the supply chain. The most widely-used method is stable isotope ratio analysis.

Scope and approach

Stable isotope-ratio signatures ($\delta^{2}H$, $\delta^{13}C$, $\delta^{15}N$, $\delta^{18}O$, and $\delta^{34}S$) play an increasingly important role in food forensics in three main areas of application: (i) detection of adulteration; (ii) assignment of geographical origin, and (iii) identification of production mode (organic *versus* conventional farming systems). Despite its success, a common limitation in food authenticity and traceability studies is the need for a readily accessible and regularly updated product reference database. This presentation deals with developing the FoodTrack database, which is organized in such a way as to enable further multivariate data analysis, GIS applications, and modelling by including parameters such as latitude (WGS 84), longitude (WGS 84), altitude(m), temperature (°C) and precipitation (mm).

Key findings and conclusions

Four different ways of evaluating the results will be presented: (i) FoodTrack data visualization in a graphical mode (maps) that enable 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 samples 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 commercial samples, discover sources of variability, predict future behaviour, and proactively avoid problems.

How Important is Calibration? An Example from Atmospheric Mercury Measurements

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The quality of a calibration method dictates the quality of the analytical results. Not only that traceability can be achieved through it, but it also gives us vital information of how our instruments respond. Lumex RA-915M is a commonly used portable gaseous elemental mercury (GEM) analyser. The device continuously monitors GEM in ambiental and polluted air in the concentration range between 0.5 and 50000 ng m-3, as stated by the manufacturer. Hg(0) is detected through atomic absorption spectroscopy (AAS) with Zeeman background correction. Although very reliable and stable, the analyser is precalibrated at the manufacturer with spyked calibration standards at much higher concentrations than the ones found in ambiental areas for Hg(0). We have developed a continuous calibration method in order to do on-site calibration that would cover the working range of ambiental GEM analysis. The results are traceable to NIST 3133 Hg(II) certified reference material. The NIST 3133 is mixed in an impinger with 3% m/V SnCl2, by the aid of peristaltic pumps. This solution is purged with N2 in order to release the Hg(0) and carry it into the analyser. This set-up provides continuous and stable signals that can be used for calibration. Calibration and measurements have been performed in different intervals of concentration, varying from 4 to 40 ng m-3, the relative combined uncertainty of measurement results varying from 6.3 to 19 % for a coverage factor of 2. In order to evaluate the analyzer and our calibration method, we have compared the results with Sir Galahad which is an automated mercury analyser with atomic fluorescence spectroscopy, and manual double amalgamation method which also detects mercury through atomic fluorescence spectroscopy. Sir Galahad and double amalgamation manual method are traceable to NIST 3133. With the calibration done at the manufacturer, Lumex RA-915M gives comparable results with the other 2 methods only at higher concentrations. At lower concentrations at around 4ng m-3, it shows an underestimation of 33%, when compared to the results calculated through our calibration method.

Isolation of oil degrading bacterial consortia by random electrostatic aggregation of cells using microfluidic approach

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Oil spills are ecological threats to marine and terrestrial environments, which are very challenging for the remediation process. Accordingly, the removal of recalcitrant polyaromatic hydrocarbons (PAH) usually requires advanced technologies for remediation. Bacteria were found to be highly effective in oil degradation and because of the complex mixture of the substrate the consortia of different bacteria are often used. However, the consortium is not always very optimal, since besides bacteria that are directly involved in the remediation also other commensal and cheating strains are present that are decreasing the efficiency. To address this issues we developed methods based of combined approach of colloid biology and microfluidics to out select the smallest and the most efficient PAH degrading consortium.

The method is based on the random aggregation of suspension of cells and immobilization in micro-sized alginate beads that are acting as microcontainers. These microcontainers enable us to prepare several 10^4 combinations of cells and therefore outperform the screening power of classical cultivation approach by several orders of magnitude.

The most efficient oil degrading consortium was selected from containers by using 2,6-dichlorophenolindophenol (DCPIP) as an colorimetric indicator of degradation of PAH. The active consortia were isolated manually using fluorescent microscopy and since microcontainers are below the 100 µm size, the continuous monitoring of the activities was performed by the flow cytometry.

Isolated consortia showed varying rates of PAH degradation showing reduction of DCPIP. The most efficient consortium was further on selected for genomic analysis.

This new approach enables rapid and efficient selection of the most optimal bacterial consortia not only for bioremediation environments contaminated either with PAH or other pollutants but also for biotechnological processes where particular multispecies processes are demanded.

Acknowledgments:

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Mercury Emission and Speciation in the Vicinity of Salonit Anhovo Cement Plant in Western Slovenia

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Atmospheric mercury (Hg) species are operationally defined as gaseous elemental mercury (GEM), gaseous oxidized mercury (GOM), and particulate bound mercury (PBM). Emitted Hg is deposited back into the environment from the atmosphere through wet and dry deposition, where the deposition rates are influenced by the Hg composition in the atmosphere. GEM has an estimated life time of about 0.8 to 1.7 years and undergoes global transport, whereas GOM and PBM have more regional and local effects. Among other Hg emission sources, the cement industry accounts for 11% of the global anthropogenic Hg emissions. In Europe, it is the second largest anthropogenic emission source after coal combustion. Mercury is brought into the cement production system from raw materials used for the clinker production, where Hg is stripped, sorbed, cycled, enriched in inner flue gases, and ultimately emitted in flue gases into the atmosphere through the plant chimney. The present study was performed to examine the influence of total gaseous mercury (TGM) emitted from Salonit Anhovo, the largest producer of cement in Slovenia, on Hg levels measured at a site (Vodarna) located 1 km downwind from the plant chimney in the prevailing wind direction. TGM concentrations in the flue gas emitted from the plant were measured using a continuous emission monitoring system (MERCEM300Z) installed at the plant kiln stack, whereas ambient air Hg speciation measurements at Vodarna were carried out with automated Tekran mercury vapor analyzer (Tekran 2537B coupled to a Tekran 1130 and 1135 speciation unit). Findings of the study revealed that plant raw mill operational conditions played an important role in concentrations of TGM in flue gases emitted into the atmosphere. TGM concentrations on average was the highest under no mill regime (49.4 µg/m^3), moderate under one mill regime (39.5 µg/m^3), and the lowest under two mill regimes (23.4 µg/m^3). Meanwhile, average ambient air Hg levels in Vodarna for the whole measurement period were 3.14 ng/m^3, 53.7 pg/m^3, and 41.9 pg/m^3 for GEM, GOM, and PBM, respectively. Atmospheric Hg speciation in Vodarna (especially GOM and PBM) coupled with plant emissions and wind data has revealed that TGM emitted from the cement plant is the major source of all Hg species measured in Vodarna. Wind blowing from the northeastern quadrant (NE, ENE) was responsible for elevated Hg levels in Vodarna, where GOM levels were highly linked to the cement plant TGM levels emitted in the flue gas. On the other hand, elevated levels of Hg species in the absence of northeastern winds indicate potential inputs from other local sources other than the cement plant as well as inputs from regional and global transport mechanisms.

Mercury Tracking via Isotopic Signature at Idrija Contaminated Site

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Idrija is a site of the world's second biggest mercury (Hg) mine. The ore deposit, mining activity and smelting locations with tailings have been, and to an extent still are, a source of Hg pollution in the area. Hg is among most toxic elements and of global concern. The world community has agreed on globally binding treaty – Minamata Convention, to protect human health and the environment form anthropogenic emissions and releases of Hg and Hg compounds. To this end, it is important to understand how Hg is transported from the pollution sources, how it cycles in the environment and what its fate in the environment is.

Mercury can be found in many forms: elemental (Hg^0), oxidized (Hg^{2+}) or it can be bound to particles (Hg^p). The most toxic are organo-mercury compounds, especially monomethyl-mercury compounds (MeHg), which bio-accumulate and bio-magnify in food webs. Once released into the environment, Hg and its compounds cycle between and within environmental compartments. Hg has seven stable isotopes. Recent advances in the measurement techniques allowed for their analysis and application to better understand the sources, transformations, and fate in the environment.

In the case of Idrija, the main environmental compartments in Hg cycling are the ore itself, the soils, vegetation, Idrijca river and air. They act either as primary sources, re-emitters, sinks and/or transport media. The use of Hg stable isotopes has been investigated for the first time at such scale in Idrija. Preliminary data indicates that proximity to the former smeltery, which is the most contaminated site in Idrija, has a significant effect of isotopic composition of the surrounding environment. Moreover, a complex link between seasonal variation on climate, different environmental compartments and proximity to Hg pollution sources has been observed.

The aim of this contribution is to present the potential and advantages of using Hg isotopes for Hg source apportionment and fate in an area heavily contaminated due to former mercury mine operation.

Monitoring of fluoride and some metals in commercial black and green teas (*Camellia sinensis* L.)

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Tea is one of the most popular and widely consumed aromatic beverages in the world [1]. It has a potential mood-enhancing effect, and consumption of tea in larger quantities may be due to its antioxidant properties beneficial in preventing cancer, hypertension, and obesity [2]. On the other hand, tea consumption may also pose a health risk [3]. *Camellia sinensis* is known to absorb fluorine and various metals from the soil and accumulate them in the leaves, from which they can be released during infusion [1,4]. Excessive intake of fluorine in the form of fluoride ions (F^-) can cause various adverse effects on different tissues, including calcified tissues, the central nervous system, thyroid gland, vascular system, and gastrointestinal tract [5]. Fluoride toxicity can be exacerbated by the presence of metals, particularly aluminium [5].

In our study, possible correlations between F^- and selected metals (Ag, Al, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, Zn) concentrations in infusions of some commercially available teas in Slovenia were evaluated. The most popular black and green teas sold in bags and their equivalents in loose form were selected for analysis. Samples were prepared by weighing 1 g of homogenized tea into the filter bag and then pouring 100 ml of boiling water over it for 5 minutes [4]. The F^- concentrations were measured using a fluoride ion-selective electrode, while metal concentrations were determined using inductively coupled plasma atomic emission spectroscopy. According to our results, the fluoride concentration (i) is higher in black tea than in green tea, and (ii) is related to the concentration of the studied metals in the infusions. The results also suggest that consumption of larger amounts of tea may even pose a health risk.

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On the importance of periodicity of environmental factors in modelling phytoplankton assemblages

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In recent years, the phenology of phytoplankton in the northern Adriatic has been studied [1, 2], but the development of a robust model for its spatial and temporal dynamics is still ongoing. Margalef's work introduced the concept of phytoplankton succession and related it to regularities and shifts in physical environmental factors [3]. Here we have attempted to extend this rough notion of periodicity to model the assemblages in two Long Term Ecological Research stations of Northern Adriatic, (000F and Acqua Alta). Using the concept of spectral decomposition of graphs, we computed the Moran eigenvector maps of our time series [4] and used them to remove the auto correlative contributions from our environmental data. We used the raw data, the residuals, and the fitted fraction to model the assemblages in the Gulf of Trieste (000F), and then used the results to predict the assemblages in a non-contiguous area, but still part of the northern Adriatic (Acqua Alta). We used the average p-values of the IndVal index [5] and the Stress-1 values [4] to evaluate the predictions. The IndVal p-values were generally lower when periodic components of the predictor variables were used, while the Stress-1 values were lower when the non-periodic part was used. The results indicate that periodicity of environmental variables is critical for structuring phytoplankton assemblages. Extreme events and climatic dysregulations, which are expected to become more frequent in the near future, could disrupt the regularity of the phytoplankton community in the northern Adriatic, with important ecological implications such as the uncoupling of trophic interactions.

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Optimization of a single particle ICP-MS method for the detection of small microplastics

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In the environment, large plastic particles are subjected to various weathering processes, which cause their degradation into very small particles, known as microplastics (MPs). MPs are defined as particles with sizes ranging from 1 μm to 5 mm, which can be further classified into small MPs <1 mm and nanoplastics (NPs) <1 μm. MNPs were already detected in almost all environmental compartments, even in the human body. The toxicity of MNPs is related to their small size, which increases their capability to cross biological barriers, to the potential leaching of toxic plastic additives and to the adsorption of environmental contaminants on the MNPs surface.

The lack of standardized analytical methods for the detection of small MPs and NPs in complex matrices hampers the knowledge of their occurrence and toxicity in the environment. An analytical method based on inductively coupled plasma mass spectrometry in single particle mode (spICP-MS), that has been so far widely used for the analysis of inorganic nanoparticles, has a potential for detecting small MPs at environmentally relevant concentrations [1]–[3]. The spICP-MS method provides information about size distribution, particle mass and number concentration.

In this study, spICP-MS instrumental parameters were optimized for different ICP-MS set-ups (by using different nebulizer types and torch injector diameters). Monitoring the signal of ^{13}C isotope in time resolved mode at very short dwell times (100 μs) allowed a distinction of background signal from particle events (Figure 1). spICP-MS analysis of 2 μm polystyrene microsphere standard showed that a combination of MicroMist concentric nebulizer and torch injector with 2.5 mm inner diameter provided the most accurate results. Particle size as well as mass and number concentration of 2 μm polystyrene microspheres determined by optimized spICP-MS parameters, were in good agreement with the values provided by the manufacturer.

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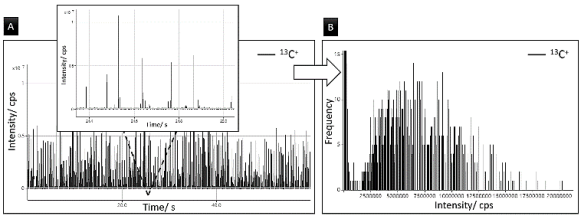

Figure 1. Time scan (A) and particle signal distribution histogram (B) of 2 μm polystyrene microspheres detected with the optimized spICP-MS parameters.

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Optimizing growth conditions of cyanobacteria and microalgae for assessment of hydrogen isotopes fractionation

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Preferences of enzymes on using lighter isotopes versus heavier can result in fractionation of isotopes. Since, water is involved in most of biological processes we can also expect preferences of lighter hydrogen isotopes in relation to the tritium and we would like to determine the extent of this biological inherent feature. It is well known that cyanobacteria and algae can split water molecules in process of photosynthesis similar as the electrolysis, but supposedly with much higher efficiency and using light as a renewable source of energy. In many of these organisms, in addition to photosynthesis, also the hydrogen can be produced by hydrogenases. Therefore, here we specified two global biochemical processes that will on one hand separate heavier protons in the first phase and then in the second one the lighter hydrogen will be expelled out, which will result in increased tritium levels in the water and biomass. Our hypothesis is that induced hydrogen fractionation during these processes would be sufficient to be explored for biotechnological purpose of removing tritium from wastewater. Since the processes must be the most efficient, several levels of optimizations are needed. For the proposed process we selected two strains of cyanobacteria (Synechococcus elongatus and Synechococcus leopoliensis) and a species of algae (Chlorella sorokiniana). For the first step, only the growth under different temperature, light and media conditions were tested. For the second step, induction of hydrogenases, the regime of environmental conditions such as frequencies of oxygen exposures and light intensities should be also elaborated. Initial results in the laboratory scale conditions show that the cyanobacteria have grown on BG-11 medium in incubator at 37 °C and under white LED light. They grew on agar plates and for the liquid media, growth was observed after pH adjustment. On the other hand, algae put in TAP medium under blue-violet LED light at room. In the next stage, fractionation potential of cyanobacteria and microalgae will be assessed by introducing tritium standard to growth medium and measuring the amount of tritium in water before and after the process via liquid scintillation counting (LSC).

Preparation of new hypervalent Group 14 based nucleophilic fluorination reagents

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Fluorine plays an important role in organic compounds due to its small size and high electronegativity. It shapes compounds to be more bioavailable, lipophilic and metabolically stable. Therefore, many recently manufactured pharmaceuticals and agrochemicals contain fluorine[1]. Since there are very few fluorinated natural organic compounds, we are forced to find alternative synthetic routes in the form of fluorination reagents. One group of potential reagents are hypervalent Group 14 based fluorides, most of which are methyl or phenyl silicon fluorides such as TASF (tris(dimethylamino)sulfonium difluorotrimethylsilicate). Among the heavier analogues of Group 14 there are even fewer representatives. To our knowledge, the only examples are limited to strongly electron-withdrawing alkyl groups[2].

In our work, we used the readily accessible 1,3-bis(2,6-diisopropylphenyl) imidazolium fluoride[3] and cesium fluoride to prepare hypervalent fluorination reagents. Using this method, we prepared fluorosilicates [IPrH][$EtSiF_4$] and [IPrH][Et_2SiF_3]. The goal of this research is to synthesise more reagents of this type based on Group 14 elements. In this way, we hope to create better alternatives for fluorination in the field of synthetic chemistry.

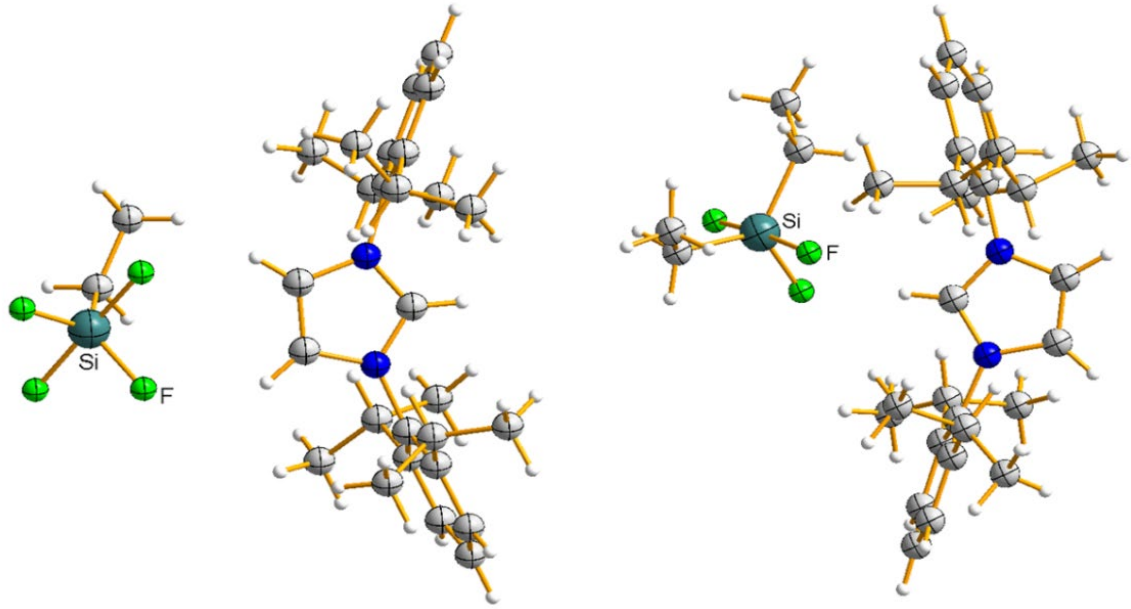

Figure 1. Examples of prepared fluorosilicates [IPrH][$EtSiF_4$] and [IPrH][Et_2SiF_3].

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Rapid detection of aqueous MeHg using cell-free transcription biosensing system

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Methylmercury (MeHg) is the most toxic mercury species and can be more easily accumulated by organisms causing prenatal nervous system and visceral damage. Therefore, rapid, cost-effective, selective, and sensitive detection of MeHg in various environmental matrices is essential. We envisage constructing a MeHg sensitive and selective biosensor using cell-free systems that allow simple, fine-tuning of circuit components stoichiometry and activation of biological processes without the use of intact living cells and provide a non-living alternative to whole-cell biosensors that could expedite their path through regulatory approval. Our work involves the expression, purification of organomercurial lyase MerB that cleaves MeHg to yield Hg2+ (inorganic mercury) which in turn would activate the cell-free biosensing system in a one-pot cascade event. We envisage using five core components cell-free transcription system: Recombinant pMerRB plasmid containing MerR regulatory operon specifically induced by Hg2+, transcriptions factors, R.N.A. polymerase, ATP. When Hg2+ induces the expression system, the expressed mRNA would be used to synthesize cDNA using complementary poly dT primers and reverse transcriptase enzyme that hybridizes onto the poly (A) priming region. The product of a first-strand synthesis (the cDNA-mRNA hybrid) is used as the template for a nick translation reaction. Ribonuclease (RNase) H produces nicks and gaps, creating a series of RNA primers used by Escherichia coli DNA polymerase I during the synthesis of the second-strand DNA. Residual nicks are then repaired by E. coli DNA ligase, and the frayed termini of the double-stranded cDNA are polished by a DNA polymerase. Standard techniques such as qPCR with forward and reverse primers and fluorescent reporter Taq-man probe (with a fluorescent reporter at (5') and a quencher at (3')) for specific sequence within the cDNA-mRNA hybrid can be used to quantitatively measure the fluorescence. The increase of fluorescence can be calculated according to the Ct values, based on the standard curve which can be used for the detection of MeHg. We hypothesize that the nano biosensor would enable us to map the Hg flux in real-time and determine the bioaccumulation and biomagnification rates of MeHg in various environmental matrices.

Key words: Methylmercury; nanobiosensor; cell-free expression system; fluorescent reporter

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Science Communication: Using podcasts for communicating mass spectrometry applications

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Public engagement in science has implications for the policies and regulations that influence scientific developments, including the financial resources allocated to research projects. Increasing public interest in scientific areas such as pharmaceuticals, genetics, geographical classification, lifestyle trends, chemical contaminants and allergen management indicates that the public is actively seeking effective media for science communication.

Podcasts are increasingly used for public engagement in various scientific and technical fields because they have a personalised style, are convenient and easy to listen to on the go and can be used to efficiently discuss concepts from an introductory to an advanced level. However, knowledge of what contributes to a podcast being an effective science communication tool is limited.

Developing this understanding will enable scientists to optimise podcast communication to maximise public engagement and understanding. The aim of this study was therefore to develop an open access guide that can be used by scientists to maximise public interest in their field of research through podcasts, trust in the content conveyed and feedback in terms of science communication.

Mass spectrometry is considered one of the most advanced and complex techniques for chemical analysis with highly technical and advanced applications in various areas of public interest, such as those previously mentioned. A series of X podcasts on mass spectrometry was created to showcase a technical invention and assess public perception.

A short-form podcast format was chosen for this research. Experts in the field of mass spectrometry were invited to participate in an informal discussion about their research and its importance to the public. The experts also talked about the impact of the research on their personal lives. A recording of these conversations was used as the main component of the focus group discussions to assess the impact on knowledge, confidence, and trust before and after listening.

Seasonal variations of $\delta^{18}O$ and $\delta^{2}H$ in tap water: case study Ljubljana, Slovenia

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Measurements of stable isotopes ($\delta^{18}O$ and $\delta^{2}H$) in tap water can provide insight into the relationship between climate, environment and consumers, as well as how the actions of people alter the water cycle. For this reason, we need to understand how interactions of tap water sources vary in space and time within the water cycle to ensure long-term sustainability. Here we report the results of a survey of $\delta^{18}O$ and $\delta^{2}H$ ratios in Ljubljana tap water supplied to the end-users from five wellfields. The research objective was to collect 100 samples over a short period with help from volunteers. Based on 182 samples collected during two sampling campaigns in March 2019 and September 2021, basic spatiotemporal characterization of isotopes in the tap water was accessed. Between the experiments, the number and surface area of each water supply area changed. However, most samples were in both cases collected at Kleče, the largest of the water supply area. Samples were mainly collected in houses from kitchens after water was left running for at least 210 s. The data collected revealed that although seasonal changes in isotope composition are small (< 1 ‰ for $\delta^{18}O$ and < 10 ‰ for $\delta^{2}H$), they are statistically significant. The $\delta^{18}O$ and $\delta^{2}H$ values in the tap water were higher in autumn and lower in spring (Figure 1). In addition, statistically significant differences were observed between the locations within the same sampling campaign. The most positive $\delta^{18}O$ and $\delta^{2}H$ were found in water from Šentvid water supply area, while water from Brest had the most negative values. The results can confirm assumptions made by domestic water supply managers about the existing division among different water supply areas.

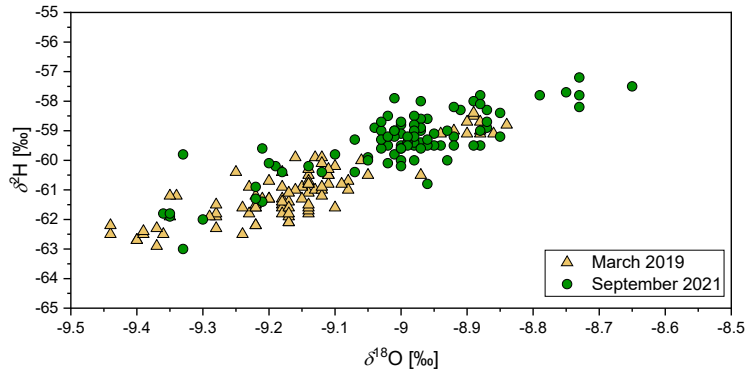

Figure 1: Relation between $\delta^{2}H$ and $\delta^{18}O$ in tap water samples collected in March 2019 and September 2021.

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Speciation of chromium in honey clover and dandelion plant using HPLC post-column ID-ICP-MS

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Chromium (Cr) is a chemical element, commonly present in the environment in rocks, soils, volcanic dust, and gases. Chromium is mostly manufactured from chromite ore and is widely used in many different industrial activities. As a consequence of its intensive use, large amounts of Cr have been released into the environment. To prevent environmental pollution, it is necessary to remediate Cr-contaminated sites. One of the promising methods for Cr remediation is the use of plants. Due to the presence of organic matter and strong reducing agents in plants, toxic hexavalent chromium is reduced to trivalent chromium and complexed by the available low molecular organic ligands such as oxalic, malic, citric, aconitic, and gluconic acids [1,2].

Seven samples from field soil with high Cr content were collected and analysed for total Cr after microwave-assisted digestion, total Cr(VI) after alkaline digestion, and exchangeable Cr(VI) applying seven successive ultrasound-assisted extractions with 0.1 mol L^{-1} K2HPO4 (pH 8). Total Cr concentrations were determined by inductively coupled plasma mass spectrometry (ICP-MS), while Cr(VI) by high-performance liquid chromatography (HPLC) post-column isotope dilution ICP-MS. Total Cr concentrations ranged from 250 to 900 mg kg^{-1}, while total Cr(VI) from 0.07 to 0.2 mg kg^{-1}, representing 0.2 to 0.3% of total Cr. Data from subsequent sequential extractions revealed, that sum of exchangeable Cr(VI) fractions gave total Cr(VI), meaning, that all Cr(VI) present in soil was bioavailable to plants. Dandelion plants (*Taraxacum officinale*) grown on filed with high Cr content were collected directly from the contaminated site, while honey clover (*Melilotus officinalis*) seeds were sown in pots with contaminated soil and the plants were collected when they were approximately 3 cm high. Plant sap was prepared according to the procedure, previously developed in our group [3]. The speciation procedure is based on the separation of Cr(III) complexes by HPLC and quantification of the separated Cr species by post-column ID-ICP-MS. The Cr complexes were determined on the basis of the retention times, while identification of ligands was performed by high-resolution MS.

Both dandelion and honey clover plants proved to be capable of high chromium accumulation. Cr speciation in both plants demonstrated some differences in the Cr species present.

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Transformation of metals using bio-catalytic cores made of multispecies aggregates

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According to the current knowledge, microbiological niches are established either by environmental factors or by the activities of microorganisms. One of the strong niche separation parameters is the oxygen level in the microenvironment, which is also an important environmental driver of controlling metabolic aerobic and anaerobic processes. It is well known that these conditions can occur naturally on a micro-scale as the structures such as biofilms or flocs are formed. However, in order to use these natural structures in biotechnological applications in remediation or bioprocessing, it is important to design and then construct such "bio-catalytic cores".

Using the method of electrostatic modification developed in our laboratory, we showed the formation of the "bio-catalytic cores" where anaerobic niches were formed enabling the growth of strict anaerobes in aerobic conditions. We showed activities of two types of such constructs composed of either single species, consisting of a facultative anaerobe *Shewanella oneidensis*, or two-species, consisting of an obligate anaerobe *Desulfovibrio africanus* and a common aerobic marine bacterium *Cobetia marina*. We determined the growth, distribution, and activity of the constructs by using fluorescent and confocal microscopy. The spatial distribution of toxic metals was determined by Scanning Electron Microscopy with Energy Dispersive Spectroscopy. Methylation of the mercury species in aerobic conditions was determined by the cold vapor atomic fluorescence spectroscopy method.

The results showed that the aggregates stay stable during the growth conditions and retained their activity for up to ten days. The aerobic methylation of Hg was confirmed in multispecies aggregates and the precipitates of reduced metals occurred in monospecies aggregates only within the anaerobic niches.

Typology for user-specific selection of the decision support system in integrated pest management

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Many decision support systems (DSS) have been developed to facilitate the sustainable use of pesticides through the integrated pest management (IPM) approach set out in the EU Directive [1]. However, selecting the most appropriate DSS is a complex decision problem, as the required information about DSS is scattered and usually not available before the end-user buys or subscribes to a DSS. To improve the selection process, we developed a set of criteria structured in a IPM-DSS typology, which we later used for a systematic description of DSS from the end-user's perspective. The typology was developed based on the structuring of IPM literature- and expert-based knowledge and provides an ordered, structured representation of concepts and terms in the form of a hierarchy. It is a semantic classification scheme and represents a knowledge map [2]. The criteria in the typology are grouped in four functional categories: (i) Challenge, (ii) Decision Problem, (iii) Decision Analysis and (iv) Final Outcomes, which are further hierarchically divided into 2 to 4 subordinate levels. The selection of the criteria was adapted for a description of DSS developed and validated for addressing decision-making problems in IPM in three European pedoclimatic zones. The typology was used to describe 80 DSS for IPM, each described by more than 55 input criteria (most detailed level of the typology). In addition to the target crop types and key pest target, the DSS typology also takes into account the geographical location (agro-climatic zones) where the DSS can be applied, the type of end-user (farmer, farm advisor or researcher), the technical requirements of the DSS, the language requirements, the affordability of the DSS and the user's preferences regarding the format for displaying the results of the DSS, to name a few. The results of the typologically described DSSs included in our study are listed in a catalogue that will be upgraded by a web-based search tool. To find the most suitable DSS, the end user will have to select the user-specific set of search criteria. The typology developed will simplify the selection process and improve the implementation of IPM practises that would lead to a more sustainable use of pesticides and a reduced impact of pesticides on the environment.

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Understanding the role of forest ecosystems in atmospheric mercury inputs to terrestrial compartment.

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Forests play an important role in global mercury cycle and represent the largest atmospheric Hg sink in terrestrial ecosystems with 500–1100 Gg of Hg stored in surface soils and vegetation. However, uncertainties associated with these estimates arise from the limited geospatial data and from the variation in reported Hg concentrations due to varying sample preparation methodology adopted. Literature suggests that dry deposition through vegetation uptake and subsequent deposition in the form of litterfall is the dominant pathway of atmospheric Hg deposition in terrestrial ecosystem however, several aspects of these intercompartmental exchanges are not well understood.

In addition to the potential explanatory variables that influence global foliar Hg uptake patterns, the use of Hg stable isotope signatures further enables understanding of the underlying mechanisms involved with changes in foliar Hg uptake mechanisms in response to seasonal climatic patterns. Furthermore, the processes of Hg retention, deposition and remobilisation can also be better explained by the changes in the Hg isotopic signatures following litterfall deposition. To this end, field visits were carried throughout the growing season for the collection of foliar samples from four forest sites in Slovenia with the presence of contrasting Hg source. Foliage samples were collected from different locations on the tree crown and were then treated in several ways to study A) the influence of methodological approaches in overall Hg determination in foliar samples and B) influence of seasonality on Hg isotopic fractionation during foliar uptake. Furthermore, experimental plots (mesocosm experiment) have also been setup to study the transformational processes during litterfall degradation with particular focus on processes of mercury retention/mobilisation patterns.

Preliminary data shows that the THg and isotopic analytical outcomes for foliar samples are influenced by the methodological approaches adopted. Samples that underwent washing procedures showed contrasting Hg isotopic signatures as well as THg concentrations although different drying methods did not affect the results significantly. Additionally, trends in Hg accumulation and isotopic signatures in foliar samples throughout the growing season will be discussed in this contribution.

Uptake and distribution of emerging contaminants by crops irrigated with reclaimed wastewater and sludge amendment

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More than 70% of fresh water is used for agriculture purposes, while population growth and climate change add to the increasing water scarcity in many regions. An alternative resource for agricultural production is the reuse of treated wastewater (TWW) for irrigation. In addition, treated sludge (TS), another water treatment by-product, could be used to fertilise agricultural areas where the pollution burden is relatively low. Both practices could contribute to improved resource management and the circular economy while reducing waste disposal costs. Although specific parameters are set for wastewater quality for agricultural irrigation (e.g., faecal coliforms, BOD, COD, TSS, turbidity,…) and sludge disposal to agricultural land (pH and heavy metals), regulations regarding organic contaminants of emerging concern (CECs) remain unregulated in both cases. These anthropogenic compounds include pharmaceuticals such as antibiotics and hormones, illicit drugs, pesticides, personal care products and industrial chemicals like bisphenols. When reusing treated wastewater in agriculture, plants could take up these contaminants and translocate them to edible plant tissues presenting a risk when consumed. In addition, their effect on plant quality attributes remains unknown.

Our goal is to understand the uptake and translocation of CECs in tomatoes (Solanum lycopersicum (L.)) grown using treated water and sludge. Three different experiments are planned, where plants will be grown under field conditions (lysimeter), hydroponic and greenhouse-controlled (pot) conditions. Pot experiments will contain peat substrate fertilised with commercial fertiliser (a), with TS (b) and with TS spiked with 30 model CECs (c). Potable water (a), spiked potable water (b), TWW (c) and spiked TWW (d) will be studied under natural and hydroponic conditions. Samples (water, soil, different plant parts: roots, leaves, fruit) will be analysed using optimised analytical methods based on ultrasonic and solid phase extraction followed by liquid chromatography (LC) coupled to tandem mass spectrometry (MS/MS). The data will allow us to evaluate selected CEC uptake and distribution under all growing conditions. In addition, we will perform a risk assessment from the consumption of TWW/TS grown tomatoes and the effect of TWW/TS on fruit quality attributes.

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Informacijske in komunikacijske tehnologije (Information and Communication Technologies)

Automated Modelling of Nonlinear Dynamical Systems Under Full and Partial Observability

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We are recently witnessing a surge of interest in machine learning methods for computational scientific discovery of laws that govern the behaviour of nonlinear dynamical systems. Typically, these would take the form of systems of ordinary differential equations. Most of the recent approaches, however, introduce new variables through the calculation of numerical derivatives (over time) of the systems variables, and then search for algebraic equations. They are therefore not capable of directly modelling systems where some of the system variables are not observed.

Biological dynamical systems are usually complex and multi-dimensional, which makes it often too expensive or even not technologically possible to measure all state variables. Consequently, we must deal with partially observed data where we have only a few measured and noise-corrupted variables. Although the dynamics of a system can in theory be reconstructed from the measurements of a single state variable (through Takens embeddings), the choice of the observables does make a difference in the difficulty of the problem of modelling the system dynamics. It also influences the understandability of the reconstructed models.

We consider the use of the ProBMoT process-based modelling tool for reconstructing models of oscillatory systems under full and partial observability. We provide to ProBMoT a library that specifies potential structures of the differential equations, as well as simulated data (full or partial in terms of systems variables). ProBMoT then performs both structure and parameter identification, using differential evolution to optimize constant parameters.

We consider three benchmark dynamical systems, including a deterministic oscillator, the chaotic Lorenz system and the Navier-Stokes equations. We examine the success of reconstructing these with ProBMoT under full and partial observability settings. Figure 1 shows some preliminary results that demonstrate the significance of measured and hidden variables. As a certain variable (in this case y) holds less information about the system, the system identification with measurements of only this variable becomes more difficult.

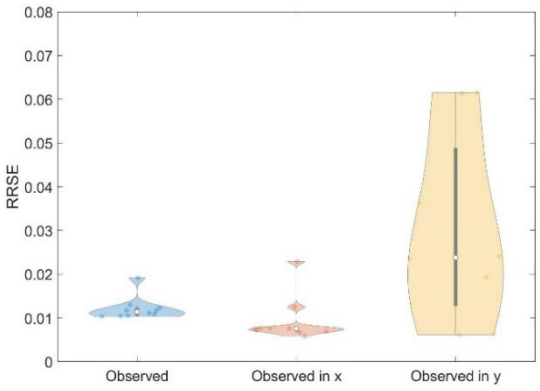

Figure 1: Success of system identification based on three observability scenarios. The relative root square error (RRSE) depicts the difference between original synthetic data of Van der Pol oscillator and its reconstruction.

BERT for Detecting Signs of Depression

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Depression, as a type of mental illness that affects a large part of our society, is one of the most complex challenges facing our humanity. Since depression is a disease that, if left untreated, can lead to serious consequences such as suicide over time, its early detection is crucial. Since people with depression typically do not open up in person very often, they often see social media as a way to express their thoughts and feelings. This trend increased rapidly with the COVID -19 pandemic due to restrictive measures that encouraged people to use social media as a means of expression. As the number of posts on social media has increased rapidly in recent years, there is a need to process them automatically to extract valuable information such as signs of depression. Increasing predictive accuracy may be critical for psychiatrists to detect the early signs of major depression to prevent further consequences. For the solution of this task I focused on exploring approaches that use a distribution of the BERT [1] model for text classification.

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Capture Point based balance controller during real-time motion imitation on the humanoid robot Talos

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Research on humanoid robotics is one of the most exciting topics in the field of robotics. However, programming such a complex system can be tedious and challenging. Learning from demonstration (LfD) is one of the approaches that can contribute to easier robot programming. It is an important research topic in the area of humanoid robotics. LfD is especially useful when the desired motion cannot be easily scripted with traditional robot programming techniques or cannot be computed by solving an optimization problem due to the lack of accurate models. The alternative is to use human demonstrations instead. This approach enables the end-users to program and teach the robot to perform movements by simply showing them to the robot. One of the basic prerequisites for LfD is the ability to capture movements performed by a human demonstrator and map them to the robot's kinematics. Standard RGB-D cameras are often used to capture human motion due to their low cost. However, the movements transferred from humans often do not result in feasible robot motion due to the differences in the human and humanoid robot kinematics and weight distribution. To successfully transfer human motions, a proper mapping function between the two different kinematic structures is needed. Stability control to prevent the robot from falling while reproducing the observed motions must also be provided.

In this work we developed a real-time motion imitation system for the humanoid robot Talos. Human demonstrations are captured using Kinect RGB-D camera and then mapped to the corresponding joint angles of the robot, respecting both joint angles and joint velocity constraints. Considering the stability problem as one of the fundamental challenges, we developed a stability controller based on the most popular stability criteria, the Zero Moment Point (ZMP). For that purpose, the robot's complex dynamics was approximated by a point mass dynamics, similar to the linear inverted pendulum mode (LIPM) dynamics. The approach assumes similar dynamics between the robot's center of mass (COM) and a LIPM, with the ZMP as a supporting point. Hence, using the dynamic relationship between the COM and ZMP, we defined a stability controller that maintain the ZMP within the support polygon. The control law is based on the Capture Point (CP) balance control approaches. Namely, introducing the CP, we can decouple the COM dynamics into a stable and unstable component where we can take advantage of the convergent component and only apply control to the divergent component of motion. The outcome is a stable trajectory of the COM, which is then related to the joint velocities using the Jacobian of the COM. We can then formulate stable reproduction of the demonstrated human motion using prioritized control, having the stability control as the primary task and imitation as a secondary task in the null space of the primary task. The result is a real-time stable motion imitation using CP-based stability control. We have shown that we can generate stable motion while imitating a human demonstrator using a LIPM-approximated model for COM. As a future work, we aim to apply motion imitation to the robot's lower body as well as learning a specific task, while improving both the achieved motion reproduction and stability.

Communicating science with art

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The intersection of art and science has a long tradition, with many consequences for the history of both art and science. Art practices, on the one hand, have always built on inventions that made scientific discoveries possible, but on the other hand, they have also provided a field in which scientific breakthroughs sui generis have been made. Primary and secondary artistic discourse has responded in different ways to changes in the contemporary civilizational paradigm, in which a broader field of 'technoculture' has emerged, in which the traditional boundaries of science, art, technology, and politics seem to be blurring. At the institutional level, many galleries, museums, festivals, and fairs have been established to promote art that focuses on the thematization of science and technology. These venues provide exposure to science for a broad audience in a way that makes it accessible to lay audiences without expertise. Artistic media allow the complex scientific concepts and their technological adaptations to be demonstrated in an efficient and compelling way, gaining popularity even among those segments of the population that have had little interest in them before. The new reality of contemporary art, with its interactive, interdisciplinary and transdisciplinary dimensions, provide a unique sensory arena in which scientific practices and discoveries can be presented, explored, problematized, and even advanced. The presentation will focus on an overview of the conceptual and contextual underpinnings of the current ways in which art is used to communicate science.

Comparison of Methods for Multi-Label Classification of Satellite Images

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Data in the form of images are now generated at an unprecedented rate. A case in point are satellite images, now available in large scale remote sensing image archives, which have attracted a considerable amount of research on image classification within the remote-sensing community. The basic task of single-target multi-class image classification considers the case where each image is assigned exactly with one label from a predefined finite set of class labels.

Recently, however, image annotations have become increasingly complex, with images labeled with several labels (instead of just one). In other words, the goal is to assign multiple semantic categories to an image, based on the high-level context present in the image. The corresponding machine learning tasks is called multi-label classification (MLC).

The classification of satellite images is currently predominantly addressed by end-to-end deep neural network (DNN) approaches, which both extract features from the images and learn classifiers from these features. After only considering single-target classification for a long period, DNNs have recently emerged that can address the task of multi-label classification. On the other hand, trees and tree ensembles for MLC have a long tradition and are the best performing class of MLC methods, but need predefined features to operate on.

In this work, we use a collection of publicly available satellite image datasets for MLC [1] to compare several DNN architectures for MLC, i.e., VGG, EfficientNet and ResNet. The architectures are trained in an end-to-end manner and used in two different modes of operation, namely, as standalone models to directly perform the multi-label classification task, and as CNN models which extract features from the satellite images. In the latter case, the learned feature representations are used with tree ensemble methods for MLC, i.e., random forests and extremely randomized trees [2].

We compare the performance of the different methods along a variety of performance measures for MLC. Of these, ranking-based evaluation measures are most relevant. According to these, the ensemble methods can further boost the predictive performance of DNNs by using the features extracted by the CNN layers of the DNNs.

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Contextual and Global Sequential Labelling Approaches to Automatic Terminology Extraction

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Terms are single- or multi-word expressions denoting concepts from specific subject fields whose meaning may differ from what the same set of words have in other contexts or everyday language. As units of knowledge in a specific field of expertise, terms are particularly useful not only for terminology extraction itself but also as preprocessing steps for other tasks such as specialized dictionary creation, machine translation, sentiment analysis, etc. In the attempt to ease the time and effort needed to manually identify terms from domain-specific corpora, automatic terminology extraction (ATE) became a crucial and challenging research task. In this research, we take advantage of contextual features from Transformers-based models (XLMRoberta) in combination with structural and global information from Graph Convolutional Neural Networks (GNNs) to enhance the performance of terminology extraction. The experiments are conducted on the manually Annotated Corpora for Term Extraction Research (ACTER) dataset [1] a collection of four domain-specific corpora (corruption, wind, equitation, and heart failure) in three languages (English, French, and Dutch). Furthermore, we evaluate our proposed hypothesis on another dataset in Slovenian covering four domains: biomechanics, chemistry, veterinary, and linguistics. The results demonstrate the benefits of our strategy, which is also a promising premise for future adaptation to less-resourced and cross-lingual settings.

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Detection of Decompensation in Chronic Heart Failure from Sounds using Machine Learning

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Chronic heart failure (CHF) is a complex clinical syndrome characterised by the inability of the heart to provide adequate blood flow to meet the metabolic demands of the body. It occurs mainly in the elderly and currently affects 64.3 million people worldwide [1]. Heart failure is associated with significant morbidity and mortality and high utilisation of healthcare resources [2]. New technologies that would improve patient management and reduce the burden on healthcare resources through HF are therefore urgently needed.

A typical pipeline for data analysis consists of signal acquisition, signal preprocessing, feature extraction and selection, and classification. The first automatic detections of heart failure and other cardiovascular diseases (CVDs) were mainly performed using data from electrocardiogram, photoplethysmogram, heart rate variability data, and clinical data. In recent years, there has been an influx of publicly available heart sound recording data sets. As a result, more and more automated methods are being developed for the analysis of heart sounds and the detection of CVD from heart sounds [3].

In this ongoing study, we are developing a method for detecting decompensation of CHF at the personal level and for early detection of deterioration of the condition using heart sound data. The data we are using is collected from the University Medical Centre Ljubljana and consists of recordings of the decompensated HF phase, a condition in which the patient requires medical attention, and the recompensated HF phase, when the patient is well and discharged from the hospital, which is usually recorded 2-5 days after decompensation. The motivation behind early detection is that early detection significantly increases the chances of bringing the disease under control, which improves the patient's quality of life in the long run. It also reduces the high medical costs associated with fighting the disease in its later stages.

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Discovering relations between integer sequences with machine learning

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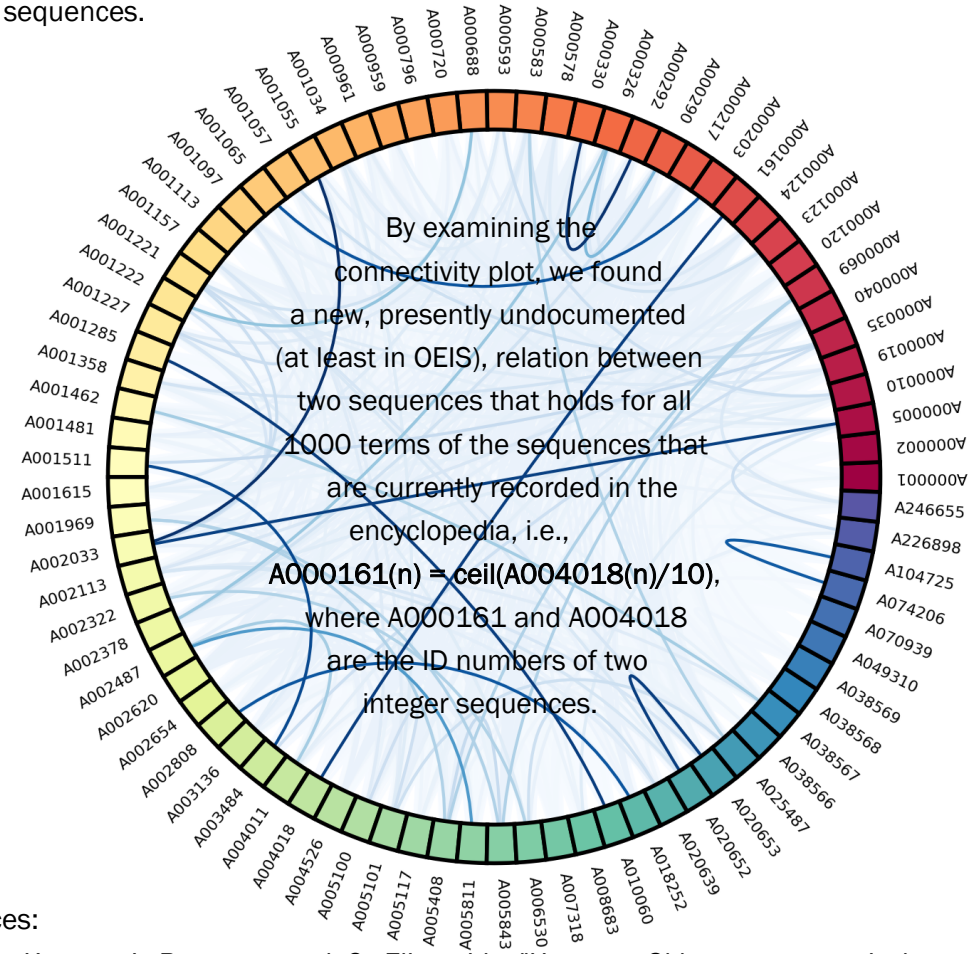
Mathematics, the mother of science, is a powerful tool applicable in all fields of science. Some of its subfields, such as number theory, that were in the past viewed as useless and recreational only, have been used in industrial applications, even if only after quite some time. In our work, we take a similarly uncertain path of discovering relations between integer sequences available in The On-Line Encyclopedia of Integer Sequences (OEIS, https://oeis.org/), without knowing in advance what the real-life implications of our results may be.

We first create a dataset from the integer sequences from OEIS, to which we then apply machine learning, and in particular an AutoML approach [1]. We combine the predictive performances of the models learned by the AutoML system with the corresponding feature importances (as determined by the permutation approach of Breiman [2] to introduce a new distance/similarity measure between sequences.



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Evaluation of an FMCW Radar as a Pedestrian Traffic Light Triggering Mechanism

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In pursuit of technologies to enable smart city infrastructure we focused on a traffic flow optimization. Specifically, we explored how to optimise pedestrian traffic light automation while also preserving the privacy of traffic participants, for which we chose an FMCW radar as a pedestrian presence sensor. In our application we used an out-of-the-box mmWave radar device with a group tracking algorithm GTRACK, that can detect the presence of multiple pedestrians at once in a predefined area. To evaluate the radar's performance, we designed two different experiments. In the first experiment, we evaluated the radar's capability to correctly respond to actions of detected pedestrians across six different scenarios. In the second experiment, we evaluated the radar's positional accuracy of detected targets (pedestrian), where we used a MoCap system with sub-millimetre accuracy as a reference. In the first experiment, the system's correct response rate was at just above 95 % across all tested scenarios. In the second experiment, the system's positional accuracy was very good in the radar's radial direction, but expectedly less so (though still satisfactory) in its tangential direction. Compared to the conventional pedestrian call button, this approach enables other, more complex functionalities. One such example is improving pedestrian road safety by extending the pedestrian call extension, if pedestrians are still present on the crosswalk.

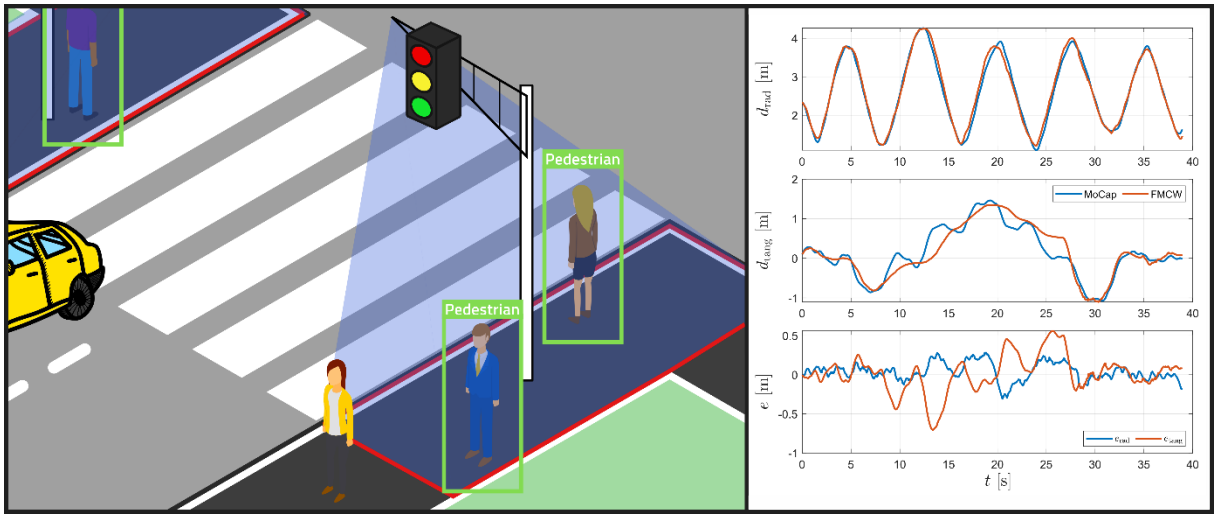

Figure 1. Left side of the figure depicts an FMCW radar monitored pedestrian crossing and the right side depicts measured positional accuracy of a single pedestrian.

Feature Selection by Combining Rankings and Dependency Graphs

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Feature selection is the process of reducing the number of input variables when developing a predictive model. It is desirable to reduce the number of input variables to both reduce the computational cost of modeling and, in some cases, to improve the performance of the model. The task of feature selection is related to the task of feature ranking, where features are ordered in terms of their (estimated) importance for predicting the target variable. Feature selection often takes the top-ranked features, but neglects feature dependencies in the process.

In this work, we propose a novel method for feature selection, which starts from a feature ranking, but also takes into account dependencies/ similarities between features. We will take feature rankings produced by the random forest [1] method of estimating variable importance. The FRANe [2] algorithm, on the other hand, produces a feature dependency graph based on these similarities.

Our idea is that selecting features based on their individual importance scores in combination with their position in the dependency graph would lead to an overall better feature selection, which will result in better predictive performance of predictive machine learning. The probability of selecting a feature will be based on its importance score (obtained from a ranking algorithm), but will be adjusted by taking into account the features already chosen and the dependency graph. We will compare our new method of feature selection with the approach that takes the most highly ranked features and ignores the dependency graph.

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Implementation of an FPGA-Based hardware accelerator for YOLOv4 convolutional neural network

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Convolutional neural networks (CNNs) have already proven to be a powerful method for solving the problem of object detection and localization. However, due to the complex architecture, they are very computationally intensive and are rarely implemented in the IoT or entry-level edge devices. On the other hand, their parallel and modular nature enables an efficient implementation of hardware accelerators. The recent development of the Field Programmable Gate Arrays (FPGAs) offers some advantages over the other hardware platforms and opportunities for acceleration at various levels. FPGAs deliver high performance through their parallelism and provide flexibility and reconfigurability for designing new hardware accelerators.

YOLOv4 is a state-of-the-art one-stage object detection algorithm and the latest revision of the YOLO architecture. The architecture reported in the original paper uses the CSPDarknet53 as the backbone, SPP additional module and PANet path-aggregation module as neck, and YOLOv3 as the head. Furthermore, it integrates advanced pre- and post-processing techniques for better performance and lower latencies. The original YOLOv4 architecture is not completely compatible with the Zynq Ultrascale+ DPU IP core therefore we modified some of its modules. We trained the CNN on the Pascal VOC dataset and using 32-bit floating-point representation accuracy of 66.8% was achieved. The usage of the 32-bit floating-point representation in the model's inference phase is often superfluous and represents the computational burden, especially on embedded devices with memory limitations. Therefore, we performed post-training 8-bit quantization for the model's parameters. The final step in transforming the model into a deployable model was compiling. Using the Vitis-AI domain-specific compiler, we optimized the models' computations and mapped them into an efficient DPU instruction stream.

We implemented the YOLOv4 CNN on Xilinx's Zynq UltraScale+ MPSoC ZCU104 development board. The hardware design was successfully synthesized and implemented using the Vivado Tools, using around 50% of the available resources of the programmable logic on the development board. The embedded ARM CPU was used to control the system and the FPGA Programmable Logic was used for accelerating computationally expensive operations. The proposed solution has a detection accuracy of 61.53%, obtaining a single-threaded performance of 14.45 FPS and a multi-threaded result of 28.48 FPS. This work showed that complex CNNs could be implemented on entry-level edge devices.

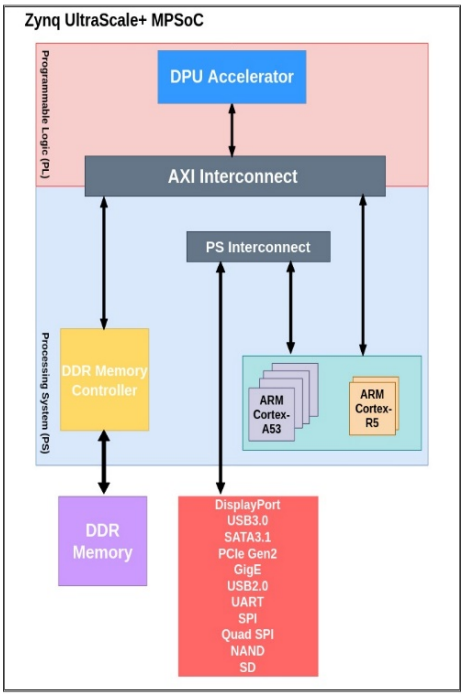

Figure 1. System block design.

Knowledge graph informed fake news detection

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Increasing amounts of freely available data both in textual and relational form offers exploration of richer document representations, potentially improving the model performance and robustness. An emerging problem in the modern era is fake news detection—many easily available pieces of information are not necessarily factually correct, and can lead to wrong conclusions or are used for manipulation. In this work we explore how different document representations, ranging from simple symbolic bag-of-words, to contextual, neural language model-based ones can be used for efficient fake news identification. One of the key contributions is a set of novel document representation learning methods based solely on knowledge graphs, i.e., extensive collections of (grounded) subject-predicate-object triplets. We demonstrate that knowledge graph-based representations already achieve competitive performance to conventionally accepted representation learners. Furthermore, when combined with existing, contextual representations, knowledge graph-based document representations can achieve state-of-the-art performance. To our knowledge, this is the first larger-scale evaluation of how knowledge graph-based representations can be systematically incorporated into the process of fake news classification.

Learning probabilities in a universal probabilistic context-free grammar for arithmetical expressions by parsing equation corpora

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Scientific research often involves the task of finding a symbolic mathematical model that best describes observed data. Models can be as simple as an algebraic equation or as complex as a system of differential equations. Equation discovery (ED), also known as symbolic regression, is the area of machine learning that develops methods for automated discovery of quantitative laws, expressed in the form of equations, from collections of measured/observed data.

ED methods often use domain knowledge to specify the space of equations they consider. LAGRAMGE [1] uses such knowledge specified in the form of context-free grammars (CFG). The recent ED system ProGED (https://github.com/brencej/ProGED) [2] uses the formalism of probabilistic context-free grammars (PCFG) in this context. Grammars specify the language of possible equation structures to consider as hard constraints (possible/impossible). Probabilistic grammars elegantly and flexibly encode soft constraints, specifying prior probability distribution on the space of possible equations (more probable/less probable).

Providing domain knowledge in the form of CFG or PCFG requires the involvement of a domain expert, who in the case of CFG has to specify the rules of the grammar, and in the context of PCFG, also the probabilities of the rules. As domain experts are not easy to come by, learning such CFGs or PCFGs from examples is highly desired. In this work, we consider learning the crucial part of a PCFG, namely the probabilities associated with the grammar rules, which we assume are given.

We start with the universal context-free grammar for arithmetic expressions used by ProGED [2] with an initial set of randomly assigned probabilities for each production rule. We then use the grammar to parse a given set of equations/ arithmetic expressions, learning the probabilities of each rule in the process. We consider two corpora of arithmetical expressions (equations), one of which is the Feynman Symbolic Regression Dataset [3] (100 equations).

According to the parsing trees used to derive the equations/expressions, we calculate the probabilities for each production rule of the grammar. We count the number of times each production rule appears in the set of parsing trees (except for rules directly resulting in terminal symbols (variables). We group the production rules by the left non-terminal symbol and derive the probabilities for each production rule as the number of appearances of a given production rule divided by the sum of such numbers for all production rules for the same left non-terminal symbol.

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Multi-Target Prediction with Dimensionality Reduction

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In this paper, we address the task of learning models for multi-target prediction with high-dimensional input (I) and/or output (O) spaces. Multi-target prediction (MTP) is employed when we need to predict multiple target attributes simultaneously and is advantageous when the target/ output attributes are related to each other. Among MTP methods, those for learning predictive clustering trees (PCTs) and ensembles thereof, e.g., extremely randomized PCTs [1] perform very well.

Solving MTP problems with very large (high-dimensional) input and output spaces is challenging as it necessitates searching large model spaces, which is computationally expensive and makes finding good models difficult. To address these issues, we will create reduced-dimensionality input (RI) and output (RO) spaces by classical methods, such as principal component analysis (PCA), as well as modern approaches, such as auto-encoders. A reduced input space can be also created by feature selection (possibly via feature ranking).

We will consider learning mappings between the reduced spaces (RI and RO) instead of the original spaces (I and O), much like Brence et al. [2]. We also consider using the reduced spaces in addition to the original ones, e.g., we may learn mappings between I+RI where the principal components derived on the input space will be used as additional features in building a predictive model for O, the original target attributes. By using the CLUS+ SW package [3] and its Python wrapper pyClus, in combination with the abovementioned dimensionality reduction methods, we will explore the influence of using the reduced spaces on computational complexity and predictive performance.

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Node embedding with SNoRe

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Graphs are useful for modelling domains such as social systems, ecosystems, and biological networks, where instances need additional information about the relationships between each other. Their complexity makes machine learning on graphs difficult, as most algorithms only accept tabular input. This issue can be avoided by using embedding algorithms, that transform graphs into tabular data. The presented approach SNoRe (Symbolic Node Representations), embeds nodes into sparse vectors with symbolic (human-understandable) features [1].

The algorithm hashes random walks from a given node into the representation of the node's neighbourhood. We compare these representations with a similarity function to obtain feature values. Because of this, feature values can be interpreted as the similarity between the neighbourhoods of the feature node and the selected node. To avoid memory overhead, only the nodes with the highest PageRank score are selected as features.

Our experiments show that SNoRe outperforms strong baselines such as node2vec and GAT on node classification, node regression, and link prediction tasks where nodes do not contain additional features [1, 2]. Additionally, SNoRe has lower time, and possibly space complexity than the strong baselines.

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Parameter optimization in models for predicting COVID-19 infections

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In the last two years, the COVID-19 epidemic has affected most countries. To keep citizens safe, governments had to take strict measures and restrict people from various economic and social activities. When deciding about the most efficient measures and their timing, they ideally consulted epidemiologists, who projected the future course of the epidemic.

Projections about future spread of disease are made using epidemiological models, which can be mathematically expressed as systems of differential equations. It is important to tune the parameters of the differential equations so that a model fits the observed real-world data the most. This is an optimization problem, and we approached it using evolutionary computation. In particular, we applied the ProBMoT approach, which considers different model structures and optimizes their parameters. This approach was proposed before [1], but it only used a single criterion to optimize the parameter values.

In our work, we use two criteria to measure the difference/similarity between the real-world data and data obtained by simulating the model — root-mean-squared error and Pearson's correlation coefficient, where the former needs to be minimized, and the latter maximized. We found this useful, because each criterion reflects a different type of information about the spread of the disease. While root-mean-squared error better approximates the number of infected individuals over time, Pearson's correlation coefficient is better at capturing the dynamics (trends) of the changes in the number of infected individuals. Using both criteria can help epidemiologists better understand the spread of the disease.

We carried out an experimental study using ProBMoT, a tool for modelling of dynamical systems. More specifically, we used the process-based domain knowledge library proposed by Tanevski et al. [1] for automated construction of epidemiological models. To optimize parameter values in the models, we used a multiobjective evolutionary algorithm [2].

Experimenting on data from five countries, we found that using only root-mean-squared error gives sufficiently good results in most cases. However, applying both criteria proved more informative for countries with several epidemic waves, because the solutions with higher correlation tend to better capture the dynamics of the spread of the disease. Thus, it is reasonable to consider both criteria when constructing models for predicting the future spread of the disease.

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Pulse Transit Time Estimation Using Multi-wavelength Remote Photoplethysmography

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Photoplethysmography (PPG) has become widely used for vital sign estimation, especially heart rate (HR), due to its simplicity, cheap implementation and unobtrusive nature. The underlying principle of skin color changes in accordance with blood perfusion has been leveraged for remote use with contact-free sensors, namely a camera. Using several PPG waveforms obtained at different locations, one can observe a delay due to blood traversing the vessels. This is known as pulse transit time (PTT) and is commonly measured using two sensors observing easily detectable reference points on the waveforms, such as the systolic peak. PTT is known to be correlated with blood pressure (BP) – stiffer blood vessels result in higher BP as well as faster blood flow, and consequently shorter PTT. The latter can also be measured between different skin layers using different wavelength light, as each penetrates to specific depth – such multi-wavelength PPG and PTT computation has already been implemented with contact sensors. However, as mentioned, PPG is obtainable remotely using a commercial RGB camera, which produces what is known as remote PPG (rPPG) reconstruction. Applying a minor modification to a commercial camera via the removal of the infrared (IR) filter on the image sensor, one can also obtain information from the near IR (NIR) part of the spectrum. We have done this to subsequently obtain three rPPG waveforms from a single measuring site – the first in the (infra)red, second in green and third in blue part of the spectrum. We have isolated the specific traces using a physical triple bandpass filter on the camera lenses (475/550/850 nm) and further subtracted the inter-channel influence to obtain pure (NI)RGB traces. Each trace originates from a different skin depth, as different light wavelengths have different penetration depth. Subsequently, we can expect a very slight delay – PTT – between the waveform reference points, as the blood requires some time to traverse from the arterioles in the deeper layer to the capillary bed in the upper layer. To capture such a short delay we used a 250-fps camera to measure the skin on the palm. Initial results show that after applying channel separation we can observe a slight PTT in the range of 0.1 s, especially between the (NI)R and G trace, as shown in Figure 1. This in turn has the potential for contact-free multi-wavelength BP estimation using a single sensor and measuring site.

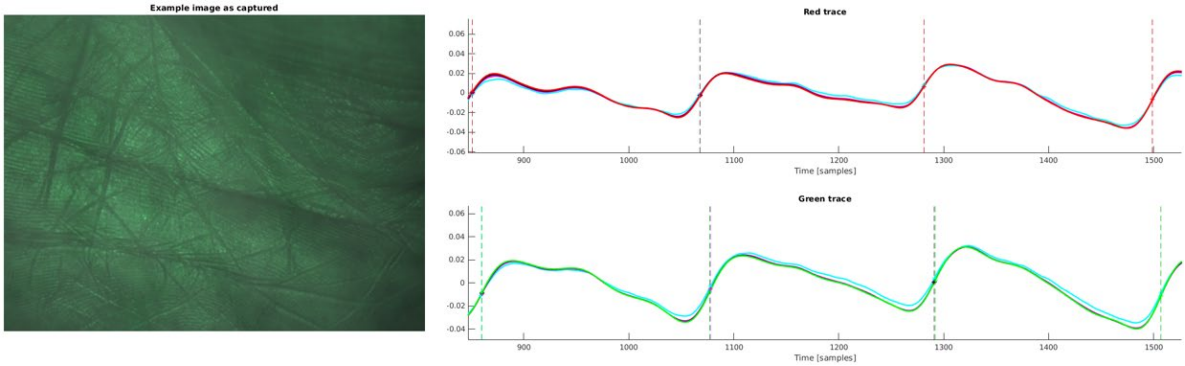

Figure 1. Observed PTT between systolic rises on rPPG waveforms at different wavelengths and skin depths.

Skill Adaptation Using Transfer Learning: Robotic Throwing

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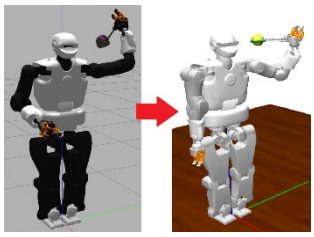

Figure 1: Source domain -(left) and target domain - (right)

Reinforcement learning (RL) made considerable progress in the past years, but mostly in simulation. This is caused by RL having relatively low data efficiency, which causes algorithms to require huge number of iterations until the task can be successfully learned. The idea of transfer learning is to use the simulation (source domain) where we can theoretically acquire infinite amounts of knowledge by RL, and apply it on the real system (target domain) with the least possible effort. In this paper we present a method of transferring the knowledge using neural networks (NN) on the example of robotic throwing action in the sagittal plane. The goal is to transfer the knowledge containing the action parameters and corresponding landing spots from inaccurate Gazebo simulation to the precisely modelled MuJoCo simulation.

The first step in our experiment was to acquire a database of executable shots in the source domain (Gazebo) and to store this knowledge in NN. We created and executed numerous examples (~1000) of robotic throwing actions and encoded them using parametric trajectory representation called Cartesian Dynamic Movement Primitives (CDMPs). Pairs of CDMP parameters (**Q**) and landing spot (**L**) were used to train NN with landing spots as input and corresponding CDMP parameters as output. We used fully-connected NN with layer sizes [2, 30, 80, 30, 101]. When the knowledge from this imprecise simulator was tested the target domain (more realistically modelled MuJoCo simulation), the initial error (shown in Fig. 2 - middle) was big. We locked all the layers of the network except the last hidden layer containing 30 neurons and started executing new shots with random desired landing spot. The newly acquired data was used to retrain the only unlocked layer of the NN. After each 10 shots, we tested the performance of the network with 20 equally spaced test landing spots and measured the precision. The final result of learning is given in Fig. 2 (right) while evolution of the average error is given in Fig. 2 (left).

With the proposed method, we managed to adapt the source domain knowledge to the target domain and achieved accuracy below 10cm in only 250 iterations. From the learning gradient in Fig. 2 (left), it is evident that this way of learning achieves fast improvements and thus has potential of being applied on the real systems. In the future, we plan to combine this method with RL techniques in order to achieve even faster adaptation.

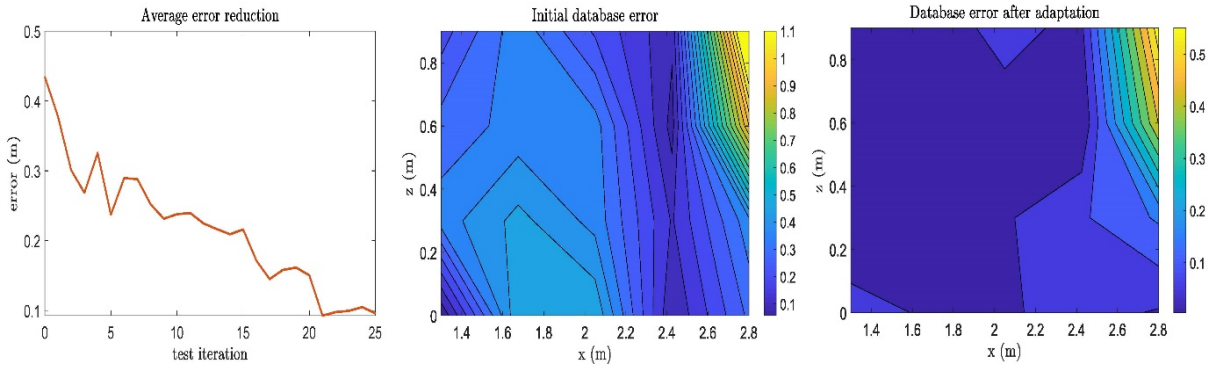

Figure 2: Average error through test iterations (left). Error before (middle) and after the adaptation (right)

Nanoznanosti in nanotehnologije (Nanosciences and nanotechnologies)

Caloric Effects in Liquid Crystal Elastomers

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Liquid crystal elastomers (LCEs) show some promising properties for developing environmentally friendlier heat-management devices. As opposed to some other materials [1], we can use LCEs to produce a moderate temperature difference under relatively small applied external fields, making them a strong candidate for solid-state heating and cooling agents [2]. There are, however, still some unknown properties of LCEs with regards to the elastocaloric effect. Namely, to create an effective and long-lasting heat-management device, LCEs would have to withstand a large number of cycles of stretching and retracting.

We report initial measurements of the fatigue of LCEs. Several LCE samples were synthesised and individually measured with a dedicated measuring device, varying various relevant parameters. Our findings show that elastocalorically efficient main-chain LCEs can withstand many stretching and retracting cycles making them a valid consideration for the cooling agent of a heat-management device. Decent elastocaloric LCEs with a cooling capability of close to 1 K per cycle can easily withstand thousands of cycles of stretching and retracting. We also observed that longer LCE samples tore significantly less frequently than shorter ones. These observations optimistically further the efforts of realising a heat-management device for real-life applications.

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Comprehensive electrochemical characterization of an LTO anode for an all-solid state thin-film microbattery

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Despite continuous improvements, lithium-ion batteries (LIB) struggle to meet the ever-increasing performance and safety requirements set by the modern consumer. All-solid-state batteries (ASSB) have recently been considered as a viable alternative, however, there are still multiple obstacles preventing broader commercialization of ASSBs. One of the major remaining challenges is the insufficient understanding of the electrochemical processes taking place on the electrode-solid electrolyte interface, which in turn leads to poor long-term battery performance. A scaled-down version of an ASSB, all-solid-state thin-film microbatteries (ATFB) have proven to be a valuable tool for studying interfacial processes, as well as finding practical use in different small-scale electronic devices. Proper characterization of such systems generally proves to be more difficult than for batteries with liquid electrolyte, as it is difficult to access the solid-solid interface without severely damaging the delicate thin film electrodes. The ability to employ *in-situ* characterization techniques therefore plays a key role in enabling a deeper understanding into the working principles of an ATFB. One of the most common *in-situ* electrochemical characterization techniques in battery research, electrochemical impedance spectroscopy (EIS) provides a non-destructive way to analyze the electrochemical behaviour of an electrode material in an already assembled ATFB.

One of the more widely used ATFB anode materials, spinel lithium titanate or LTO ($Li_4Ti_5O_{12}$) exhibits little volume change (0.2–0.3 %) and high stability during electrochemical cycling, which makes it an excellent candidate for use in ATFB model systems [1]. Our research encompasses the fabrication of a thin-film LTO anode with the pulsed laser deposition technique, and its subsequent structural and electrochemical characterization in different ATFB configurations, including a full-cell ATFB. One of our main goals is to perform a somewhat broader EIS characterization of such a system by employing a transmission line model (TLM), which is commonly used in LIB impedance modelling. Such a model could be used to obtain certain physically meaningful battery parameters, which are otherwise difficult to extract using less broadly applicable equivalent circuit models [2].

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Design of a Smart Phone Self-Charging Device Based on Permanent Magnets

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Mobile electronic devices, particularly smartphones, are indispensable part of everyday life. A smartphone is no more just a communication device but it is rather a tool to help people in various areas, such as online classes and meetings, internet banking, web browsing and social media platforms. One of the weakest parts of a modern smartphone is a limited capacity of the battery. This is supposed be sufficiently high, whereas the charging times should be as short as feasible. In spite of a huge progress in this field, it makes sense to recharge a phone whenever it is possible. For this reason, it is convenient to take the advantage of converting any type of energy into electricity, for example, during walking off the phone carrier. One possibility is a self-generation system based on magnetic induction caused by the oscillation of a permanent magnet in a coil. We focus on the design of a magnet, which must be suited for low-cost production methods such as additive manufacturing. It is shown that a homogeneously magnetized, non-uniformly shaped magnet is just as efficient as a complicated magnetization configuration.

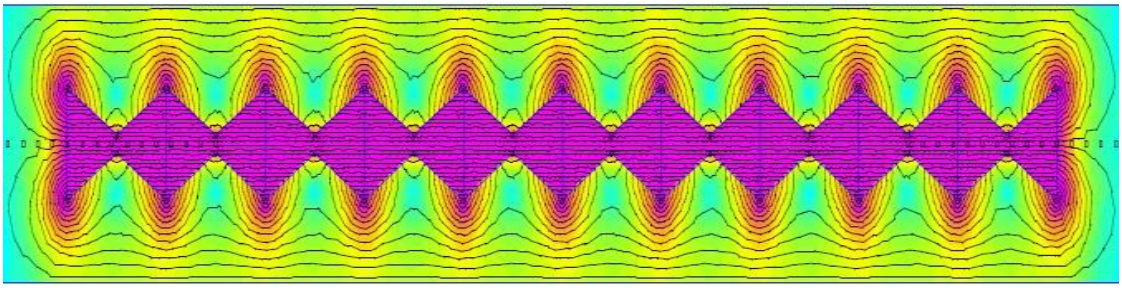

Fig.1. The calculated flux lines around the magnet in the equilibrium position.

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DFT study of dry reforming of methane at Ni/CeO_2 and Ni/Mn_xCeO_2 catalysts

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Methane dry reforming (MDR) reaction converts CH_4 and CO_2 to syngas (a mixture of H_2 and CO) that can be further converted into valuable chemicals. Both CH_4 and CO_2 are very stable molecules, hence their decomposition is highly endothermic. Sagar and Pintar [1] researched MDR at Ni nanoparticles on ceria (CeO_2) and Mn-doped ceria (Mn_xCeO_2) supports. The Mn_xCeO_2-supported catalyst was found superior to the CeO_2-supported one. A puzzling difference between the two catalysts, revealed by vibrational spectroscopy, is the peak at 2020 cm^{-1} observed only on the CeO_2-supported catalyst. On this basis, a different mechanism was proposed on each catalyst [1].

To explain the origin of the 2020 cm^{-1} peak, we performed vibrational DFT calculations and calculated vibrational modes of species involved in MDR reaction, including different reaction intermediates. Calculations revealed that the 2020 cm^{-1} peak is due to CO adsorbed on metallic Ni nanoparticles. Since CO is the product of MDR, the lack of this peak on Mn_xCeO_2-supported catalyst suggests that Ni nanoparticles oxidize thereon and, consequently, the frequency of adsorbed CO changes.

To explore this scenario, we performed transition-state DFT calculations for decomposition of CH_4 and CO_2 on Ni(111) and NiO(100) surfaces, representing limiting cases of the least and the most oxidized Ni particles. Results reveal that the MDR reaction is viable on both surfaces, indicating that the reason for different vibrational spectra obtained on the two catalysts could be higher oxidation of Ni particles on the Mn_xCeO_2-supported one. This also explains the observed higher coke resistance of the Mn_xCeO_2-supported catalyst because coke formation is less favored on NiO than on Ni surfaces.

This study has been performed in collaboration with V. T. Sagar and A. Pintar from National Institute of Chemistry.

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Effect of infill strategy on mechanical properties of parts prepared by thermoplastic 3D printing

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Ceramic additive manufacturing (AM) allows shaping ceramics with a level of complexity unprecedented by conventional methods. One of the many available ceramic AM processes is thermoplastic 3D printing (T3DP), recently referred to as Multi Material Jetting (MMJ), where a thermoplastic ceramic feedstock is deposited in the form of droplets, which merge to form lines that merge further to form layers. This building logic allows modifying the direction of deposition of droplets and lines, which is commonly known as infill strategy. Changing the infill strategy affects the final properties of the parts, particularly the mechanical properties. Although 0°, 90° and ±45°infill strategies have been studied for different AM methods, the effect of different infill strategies on parts prepared by T3DP is yet unknown.

In this study, we aim to understand the effect of different infill strategies on the final mechanical properties and flaw types present in parts prepared by T3DP. For this purpose, we prepared bending bars with 0° and 90° infill strategies as well as a combination of both. Rectangular bending bars were printed using a wax-based zirconia suspension, debinded and sintered to reach high theoretical densities above 99% for all parts. In addition to microstructural analysis and phase characterization, mechanical properties of sintered parts were studied by 4-point bending test, Weibull analysis and SEM imaging to understand the strength and reliability of parts as well as flaw types present in parts with different infill strategies. Combining infill strategies did not result in better final properties, it was shown that characteristic strength of 624 MPa and a Weibull modulus of 6.02 was obtained for these parts, while 0° infill strategy was found to be the best option for strength and reliability where a characteristic strength of 700 MPa and a Weibull modulus of 6.98 was achieved. It was also shown that parts prepared by T3DP had competitive values of strength to those achieved by commonly used ceramic AM techniques, fused filament fabrication and stereolithography.

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Exploring glioblastoma therapeutic resistance in a patient-derived organoid model

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Glioblastoma is the most common primary brain tumor in adults. Despite established treatment regimens including surgical resection, radiotherapy and chemotherapy with temozolomide (TMZ), the prognosis of patients is poor. The tumors almost inevitably acquire therapeutic resistance and recur. In the present study, we aimed to explore the mechanisms of glioblastoma resistance to irradiation and TMZ. To account for possible effects of stromal cells in the tumor microenvironment, we used a patient-derived organoid model established from patient tumor tissue [1]. Cellular composition of the organoids was analyzed by immunofluorescence staining, which revealed the presence of glioblastoma stem cells and differentiated cancer cells, endothelial cells, and immune cells including macrophages, microglia and lymphocytes (Fig. 1). Gene expression profiles and subtypes were compared between organoids and original tumor tissue to further evaluate the relevance of the model. Organoids from 11 patients were subjected to a single dose of irradiation (10 Gy), a one-week treatment with TMZ (50 μM), or their combination. None of the treatments significantly affected organoid viability and invasion. The response to therapy was further examined at the level of gene expression. Among a number of genes related to tumor microenvironment, epithelial-mesenchymal transition, glioblastoma subtypes, stemness, DNA damage response and cell cycle, several targets were differentially expressed in the organoids after treatment. Our results shed light on potential mechanisms of therapeutic resistance in glioblastoma.

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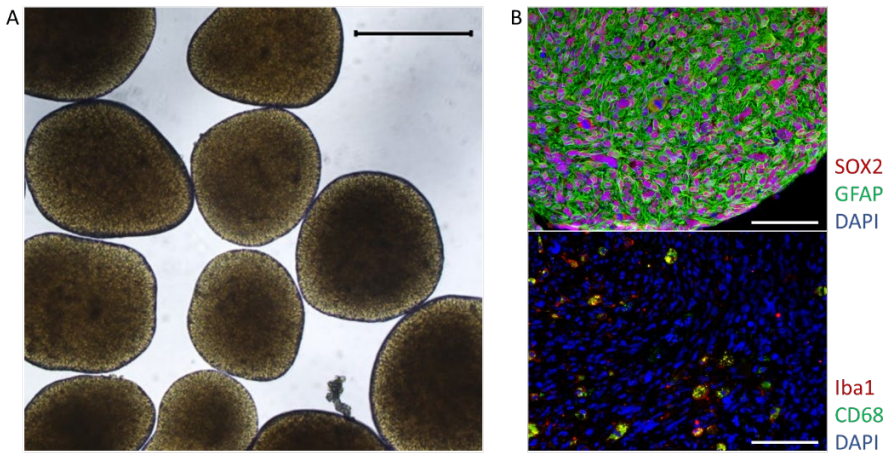

Figure 1. Glioblastoma organoids. A) Glioblastoma organoids in culture. Scale bar: 500 μm. B) Immunofluorescence staining of selected marker proteins in glioblastoma organoid sections. SOX2 – glioblastoma stem cells, GFAP – differentiated glioblastoma cells, Iba1 – microglia, CD68 – macrophages. Cell nuclei are stained blue. Scale bar: 100 μm.

Genome editing for phytoplasma-resistant grapevine

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Grapevine yellows diseases, caused by phytoplasma, are becoming an increasing problem in viticulture, as no effective cures are available. Effective prevention consists mainly of spraying against its insect vector, which is expensive and puts a burden on the environment. Producing disease-resistant varieties is the most cost-effective and sustainable option to mitigate the impact of this disease. Different grapevine cultivars can be more or less susceptible to grapevine yellows diseases, but no cultivar is currently known to be completely resistant. Therefore, even classical breeding techniques may not be sufficient to produce a phytoplasma-resistant grapevine variety. However, genome editing technologies are opening new possibilities for introducing disease resistance into plants.

With genome editing methods, such as the CRISPR-Cas9, it is now possible to make very precise changes in any given gene without affecting the rest of an organisms' genetic code or inserting foreign DNA. If we can identify genes that are involved in the susceptibility to a certain plant disease it is possible to use these new technologies to produce resistant crops that maintain the rest of the properties of an elite cultivar, which is a major concern in grapevine.

When looking for potential targets for increased resistance, one of the best candidates are susceptibility genes. These genes are hijacked by pathogens upon infection in order to promote their own fitness. Changing them can potentially remove the ability of the pathogen to exploit them. In our recent study we investigated the transcriptomic response of grapevine cv. Zweigelt to '*Candidatus* Phytoplasma solani' infection in the field [1]. Of specific interest were two members of the *DMR6* gene family, which have demonstrated an increased expression in infected plants, typical of susceptibility genes. Members of this family are presumed to be negative regulators of immune response in plants and have already been demonstrated to be involved in susceptibility to other diseases in grapevine, as well as in numerous other plant species.

We hypothesize that one or both of the genes identified in our study contribute to phytoplasma susceptibility in grapevine and that removing their function will result in resistant grapevine cultivars. In our further research we hope to use the CRISPR/Cas9 system to produce foreign DNA-free genome edited grapevine with loss of function in these susceptibility genes. These results will help us to understand the mechanisms of phytoplasma infection in grapevine and may also provide a commercially interesting variety.

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Genome informed design of real-time polymerase chain reaction for detection bacteria

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Real-time polymerase chain reaction (qPCR) is a sensitive and specific diagnostic tool that allows rapid and culture-independent detection of microorganisms. It is particularly useful for the detection of bacteria that are difficult to isolate and detect using microbiological methods due to their fastidious growth under laboratory conditions. An example of such a bacterium is *Xylophilus ampelinus*, a plant pathogen that causes bacterial blight of grapevine. It was first described in Crete (Greece), but has been found in many Mediterranean countries as well as in South Africa and Japan [1, 2]. Diagnostic tests currently used to detect *X. ampelinus* sometimes lack specificity for reliable detection. To address this problem, we decided to design new primers and probes that specifically bind to the nucleotide sequence in the genome of *X. ampelinus*. We used publicly available genomes and nucleotide sequences from RefSeq and GenBank databases to identify species-specific nucleotide sequences. To identify such sequences we used online bioinformatics tool RUCS (Rapid identification of PCR primers for unique core sequences) [3]. To perform the analysis, we needed two data sets. The first set contained nucleotide sequences belonging to *X. ampelinus*. The second set contained sequences from closely related bacteria to which the primers should not bind. This set contained genomic sequences of other bacterial species in the genus *Xylophilus*. RUCS identified unique core sequences, present only in *X. ampelinus*. The Primer Express 2 program was used to design primers and TaqMan probes that bind to unique core sequences. The melting temperature (T_m) was set at 58 - 60 °C for the primers and 10 °C higher for the probes. The length of amplicons ranged from 50 to 150 base pairs. The Basic Local Alignment Search Tool (BLAST) was used to identify non-specific binding of the primers and probes. The ten primer and probe sets with the highest scores were selected for further laboratory testing. DNA extracted from the target microorganisms at known concentrations is used to determine the efficiency of amplification and sensitivity of the assay. Various reagents and amplification conditions will be tested to find the optimal reaction mixture and temperature profile for qPCR. Results will also be compared to those obtained with currently available assays.

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How can we fabricate passive electronic components in a greener way?

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Going green and more efficient is the key to better living. In the electronic era, dielectric ceramics are widely used in wireless communication systems and various electronic devices. Even so, their large-scale production still requires high temperatures and negatively contributes to high energy consumption. One of the incentives to reduce the processing temperatures is Room Temperature Fabrication (RTF) of "upside-down" composites, which constitute of high loading of functional ceramic filler and a small amount of binder admixed to the ceramic particles in the form of a solid and saturated aqueous solution[1]. In this way, bulk ceramic upside-down lithium molybdate-strontium titanate (LMO-ST) composites were fabricated at room temperature [2]. As the LMO binder is deposited on the surface of ST filler particles during pressing and drying, composites densify. In our research, we were stepping through different stages of the process, to gain a deeper insight into and optimize the densification process. Up-to-now composites resulted in a sufficient binding with 76 to 85% relative density, relative permittivity in the range of 65–120 and dielectric loss tangent values of 0.002–0.05 at 1 MHz. By the fact that the connectivity of a composite plays a key role in its properties, we shed light on the investigation of the surface modification of ST, wetting, and the crystallization of the LMO. Results of mathematical predictions highlighted the influence of remaining porosity which has a detrimental effect on dielectric and mechanical properties. By addressing this, the fiber-reinforcement and impregnation post-treatment are under investigation. The implementation of different materials in multicomponent composites widens the range of functional properties prominent for electronic applications.

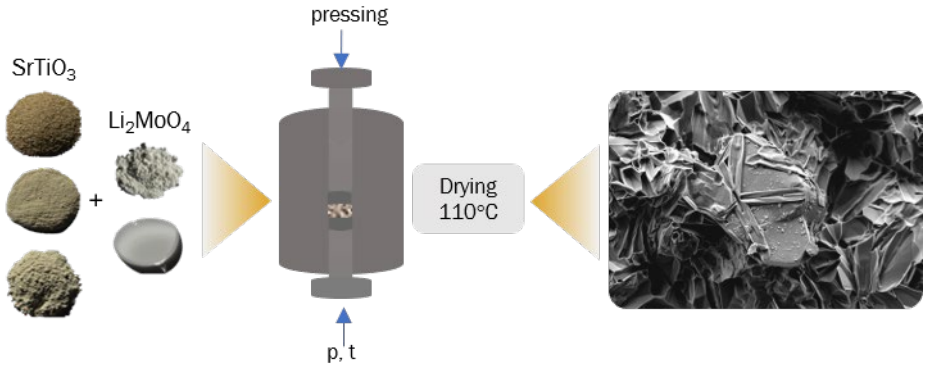

Figure 1. RTF processing of LMO-ST composites.

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Improved analytical approaches for defining vector genome integrity in Adeno-associated viral based gene therapeutics

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In recent years, adeno-associated virus (AAV) vectors have been widely used for delivery of therapeutic DNA in order to fight acquired and genetic diseases. With the increasing number of clinical trials and approved AAV-based gene therapeutics, regulatory agencies have become even more focused on the safety and efficacy of these drugs. Currently, two major issues are the integrity of vector genomes and the presence of DNA impurities (e.g., host cell DNA and plasmid DNA) that may pose a safety risk, if not well defined or removed.

In our work, synthetic DNA containing the major components of the AAV genome was used to develop a multiplexed droplet digital PCR (ddPCR) approach to comprehensively assess the integrity of the vector genome. The synthetic DNA was fragmented with various restriction enzymes to obtain different DNA fragments. Bio-Rad's QX One ddPCR system was compared with the Qiagen's QIAcuity dPCR system to evaluate their advantages and disadvantages. Next, we developed a protocol for AAV sample preparation and sequencing using the MinION platform from Oxford Nanopore Technologies. Theoretically, this sequencing approach allows us to sequence the full-length DNA molecules present in the samples, which could help us accurately determine the integrity of the vector genome.

Similar results were obtained with both tested dPCR systems when fragmented synthetic DNA was used as starting material. The cost efficiency and specific software features proved to be a major advantage of the Qiagen's system.

Establishing the protocol for DNA extraction and sequencing of AAV genomes using the MinION platform was more challenging than originally anticipated. The required concentration and amount of AAVs for optimal library preparation can be difficult to obtain, but we were successful when adding lambda phage DNA to a smaller amount of AAV DNA. The results showed that the sequencing technology used is biased toward shorter DNA fragments and that vector genomes block pores during sequencing, resulting in lower data output. Nevertheless, we were able to detect some differences in the size distribution of DNA fragments between the tested samples. Next, we detected relatively long DNA impurities derived from plasmids used in AAV production. The presence of plasmid DNA is usually determined and quantified by single-target qPCR, which cannot determine the length of these molecules. Our experiment has shown that the plasmid DNA in the viral capsids actually contains full-length antibiotic resistance genes, which may affect the safety of these drugs.

Increased cathepsin X activity in glioblastoma: The effect of its inhibition and the interplay with γ-enolase

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Proteases, including cysteine cathepsins, are functionally involved in many processes of cancer progression. While upregulation of the lysosomal cysteine carboxy-peptidase cathepsin X has been associated with neuroinflammatory diseases, the role of cathepsin X in cancer, particularly glioblastoma (GBM), remains unknown. In this study, cathepsin X expression and activity were found to be upregulated in recurrent and *de novo* GBM tissues compared with low-grade gliomas and non-tumor brain tissues. In addition, immunofluorescence staining confirmed the localization of cathepsin X in GBM cells as well as in tumor-associated macrophages and microglia. Subsequently, the effects of potent irreversible (AMS36) and reversible (Z7) selective cathepsin X inhibitors were examined *in vitro*. The inhibitors impaired the viability and proliferation of patient-derived GBM cells as well as macrophages and microglia, cultured in conditioned media of GBM cells. Previous studies identified γ-enolase as one of the substrates of cathepsin X carboxypeptidase activity in the brain. The correlation between the high proteolytic activity of cathepsin X and C-terminal cleavage of γ-enolase and colocalization of cathepsin X and γ-enolase was also observed in GBM tissues, preferentially in GBM-associated macrophages in microglia. These data suggest the possible role of cathepsin X in GBM progression and represent a potential target for therapeutic approaches against GBM [1].

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MR imaging and numerical simulation of dendrite growth in lithium batteries

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Modern lithium-ion batteries are light, energy dense and relatively cheap, however, further development towards using lithium metal as anode material is being staggered by the insufficiently understood problem of lithium dendrite growth [1]. During the recharging phase, spiky, needle-like microstructures called dendrites are formed on the anode, causing a rapid decrease of the cell's capacity. If the dendrites happen to reach the other electrode, the cell is short-circuited, causing a thermal runaway, which is a major safety hazard [2,3]. Understanding how such growth is affected by the electric currents inside the cell is a crucial step towards furthering the development of lithium batteries. Our aim is to develop a stochastic model, that approximates the macroscopic dendritic growth and compare it to 3D images we obtain with MR imaging (fig 1). The main mechanism used for simulating lithium deposits is called diffusion-limited aggregation [4]. Although diffusion is not the main transport method of the system, it can be modified to consider potential fields, such as electric, magnetic, gravitational, etc. The goal of this contribution is to form an empirical link between calculated electric current distributions and the probability of lithium deposition in the simulation model. These simulations could potentially prove beneficial in the development of commercial rechargeable lithium batteries.

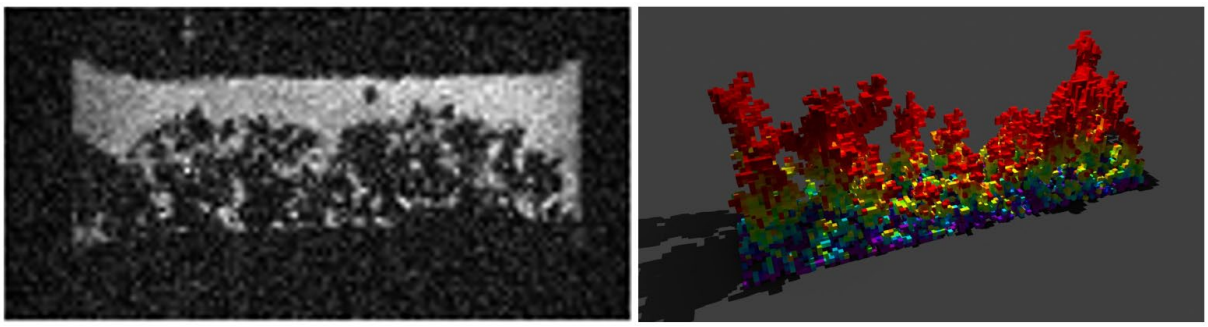

Figure 1. MRI slice of a battery model exhibiting dendrite growth (left) and simulation results of Li dendrite growth (right).

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Optimization of Semiconductor- Superconductor nano-systems for the development of Andreev qubits

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Two-dimensional electron systems confined near the surface of narrowband semiconductors have piqued interest due to their ease of integration with superconductors, allowing for new hybrid device systems. These hybrid systems lay the foundations of a radically new solid-state platform for scalable quantum computing based on Andreev quantum bits (qubits). These Semiconductor-superconductor hybrid systems resulting in Andreev qubits are among the most promising candidates, as high-quality superconducting thin films with transparent interfaces to a low-D semiconductor will improve coherence time as well as offers strong qubit-qubit coupling [1,2]. InAs 2D electron gases (2DEGs) are the ideal semiconductor systems due to their vanishing Schottky barrier; however, their exploitation is limited by the non-availability of commercial lattice-matched substrates [3,4].

In this work we have demonstrated that in-situ growth of aluminium films on near-surface InAs 2DEGs can be grown by Molecular Beam Epitaxy on GaAs substrates with quality comparable to state-of-the art growth on InP despite 7% InAs/GaAs lattice mismatch [5]. Adaptation of the metamorphic growth protocol has allowed to reach low-temperature electron mobilities around 5X10^4 cm^2/Vs in InAs 2DEGs at 10nm from the surface. In-situ growth of Al films resulted in single crystal thin films. Atomic force microscopy (AFM) and X ray reflectivity (XRR) showed that Al deposition is conformal to that of the underlying semiconductors, which preserved the cross-hatched pattern typical for metamorphic growth. Resistivity as a function of temperature was comparable to the best Al layers on GaAs and superconducting proximity effect was observed in a Josephson junction. The growth protocol developed could thus set a new standard for the fabrication of Andreev qubits on GaAs technology.

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Permeability of vacancy defects in graphene for diffusion of H_2 and O_2

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It was recently shown that deposited graphene-oxide (GO) and reduced graphene-oxide (rGO) layers on Pt surfaces display selectivity toward oxygen reduction reaction (ORR) and hydrogen oxidation reaction (HOR). In particular, experiments revealed that rGO@Pt selectively inhibits ORR in aqueous electrolytes while having almost no impact on HOR activity [1]. This selective behavior was associated with intrinsic defect structures in the rGO layers and wrinkles formed between individual GO and rGO flakes on top of the Pt electrode [1]. To provide complementary insight into the role of defects in graphene layers and the role of crevices between individual graphene flakes, we have undertaken a computational study of diffusion of hydrogen on oxygen through vacancy and crevice defects in the graphene. Molecular modeling, based on density functional theory and periodic boundary conditions, surprisingly reveals that a relatively large vacancy defect in the graphene layer is required even for the smaller H_2 molecule to diffuse through the layer without a significant energy barrier, whereas for the larger O_2 molecule the required size of the vacancy is even larger.

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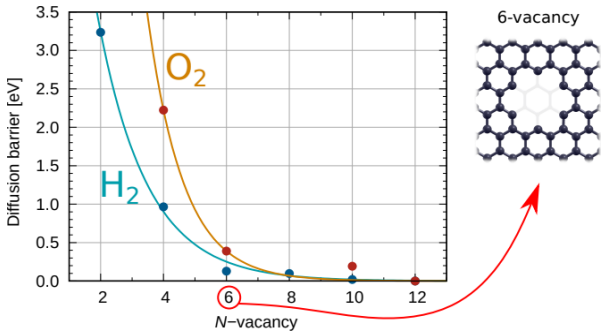

Figure 1. The diffusion barrier as a function of the vacancy size in a graphene sheet for the diffusion of H_2 and O_2 molecules. The size of a vacancy is expressed as *N*-vacancy, where *N* is the number of missing C-atoms.

PVD Coatings for High-Temperature Applications

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Physical vapor deposition (PVD) coatings protect industrial machining tools against wear. Several industrial processes are held at high temperatures, which can damage even the coatings. Therefore, it is important to understand the properties of PVD coatings at high temperatures. However, there are many problems with measurements of mechanical and tribological properties at high temperatures and most of them are connected with different properties of measuring equipment at elevated temperatures, which can alter the results significantly.

High-temperature hardness is measured with nanoindentation using the Oliver-Pharr method [1]. However, it is complicated, due to constant changes in the coating and the measuring system. One of the problems is achieving an isothermal contact which means a minimal flow of heat between the sample surface and the indenter and minimal thermal drift (changes in the normal operational behavior of indentation because of the changes in ambient temperatures) [2].

The next problem is tip degradation. Oxidation, softening and especially mechanical wear (blunting) when measurements are done on hard materials, all correspond to the tip degradation. Diamond is the most common tip material, but it starts to oxidize above 400 °C [3]. Softening is especially problematic since the hardness of diamond drops by 50 % at 800 °C. Therefore, the reliability of results is questionable, because for reliable results the difference between the hardness of the sample and the indenter material has to be substantial and PVD coatings usually have high hardness [4].

There is still much to explore in the field of measuring high-temperature hardness and other properties. More work should be put into the development of reliable equipment and methodology.

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Red blood cell derived vesicles for gene therapy and theranostics

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Although nanomedicine is, nowadays, a staple in drug development, there's still urgency of new carriers for specific applications. In particular, cell-derived objects, such as exosomes and extracellular vesicles [1] have been proposed as alternatives to traditional dendrimeric and liposomal nanocarriers for theranostics and precision medicine applications. Red blood cells are promising starting material for such purposes: they possess on their surface CD47, a "don't eat me!" marker for macrophages, escaping therefore immune system recognition. Erythrocyte-membrane vesicles (EMVs) can be produced via shear stress processes over hemoglobin- depleted erythrocytes, consisting of merely double layer, integral proteins, and cytoskeleton. We already demonstrated superiority of EMVs as carriers for t2 MRI contrast agents [2] and for cyanine dyes in case of photothermal therapy and imaging [3]. Currently, we are investigating their suitability as therapeutic nucleic acids carriers (mRNA, siRNA, anti-sense oligonucleotides) [4].

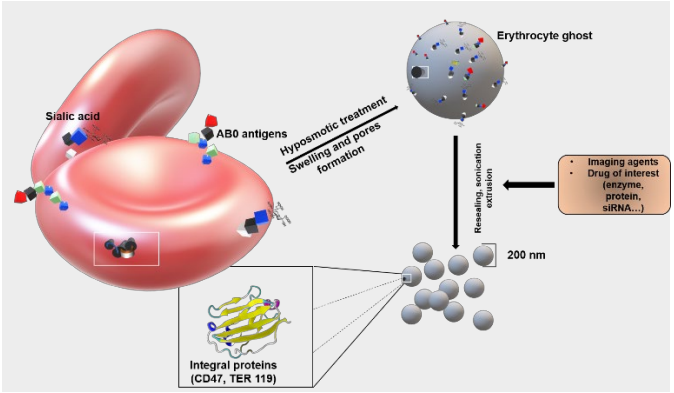

Figure 1 Schematic representation of EMVs preparation

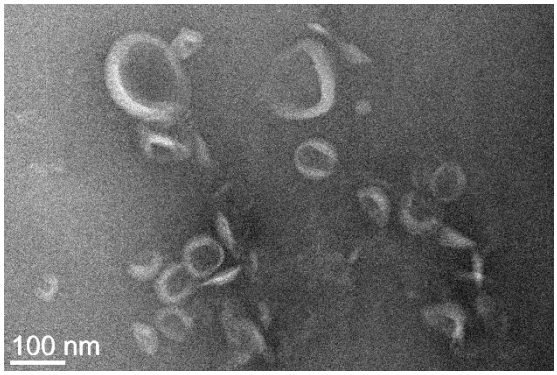

Figure 2 Negative stain TEM micrography of EMVs.

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Space charge contributions to the dielectric response and breakdown strength of high-temperature polyetherimide/polyimide blends

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Capacitors are an indispensable part of modern electronics and electrical power systems. Compared to ceramics, polymer-film capacitors are inexpensive and can be produced in a variety of shapes. One of the major challenges in developing dielectric polymers is realizing high energy density while maintaining low dielectric losses. The composite approach, in which conductive particles are dispersed in the dielectric matrix, effectively increases the dielectric permittivity but also boosts the losses [1, 2]. An alternative approach is operation under higher electric fields, i.e. increasing the electrical breakdown strength without increasing the dielectric permittivity.

Phenyl groups are fundamental chain components of many high-temperature polymers and, depending on the polymer's molecular structure, delocalized electrons in these groups may exhibit a partially positive or negative charge. Blending of appropriately matched polymers can thus result in high chain packing density and a reduction of accumulated space charges that initiate breakdown at lower electric fields. Indeed, a preliminary study showed an enhancement of the breakdown strength in blends of polyetherimide (PEI) with polyimide (PI) due to strong electrostatic interactions between the phenyl groups of different polymer chains [3].

To further investigate the influence of the interchain interactions on the dielectric response, we prepared several PEI/PI blends by solution casting method and performed high-resolution dielectric measurements over broad frequency and temperature ranges. While the dielectric permittivity of the blends is almost identical to that of pristine PEI and PI, their electrical conductivity is significantly (up to 40%) lower. Additional low-frequency measurements corroborated that blends with lower intrinsic electrical conductivity accumulate less space charges. Moreover, the temperature-dependent measurements of both annealed and non-annealed samples revealed the influence of aging processes and, particularly, absorbed water on the dielectric permittivity and relaxation processes in PEI/PI blends. This finding indicates that the annealing procedure, i.e. high-temperature treatment, could also influence the breakdown strength, which is going to be the subject of our further study.

Our results confirm that molecular engineering of high-temperature polymers can reduce the amount of accumulated space charges and consequently enhance the electrical breakdown strength, making polymer-film capacitors even more attractive for further development.

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Steering the Hydrothermal Topotactic Epitaxy of $SrTiO_3$ on $Bi_4Ti_3O_{12}$ Platelets by Supersaturation

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Engineering of functional materials, including photocatalysts, with improved properties, is possible when it is based on a detailed understanding of the reaction mechanisms and nucleation-crystallization processes. We are attempting to contribute to solutions for energy-related problems by the development of H_2 evolution photocatalysts based on heterostructures with improved charge carrier separation. Due to the favorable band edge positions and the similarity of crystal structures, the proposed candidates are epitaxially intergrown $SrTiO_3/Bi_4Ti_3O_{12}$ heterostructures. However, their formation under alkaline hydrothermal conditions is not straightforward and an understanding of the transformation process is needed. X-ray diffraction and electron microscopy techniques help us to understand this process, which occurs by $Bi_4Ti_3O_{12}$ dissolution and $SrTiO_3$ epitaxial growth until complete transformation into $SrTiO_3$ platelet. Nanoscale examination of the individual phases and the $SrTiO_3/Bi_4Ti_3O_{12}$ interface using a high-resolution transmission electron microscope (HR STEM) enabled us to determine the {110} $Bi_4Ti_3O_{12}$ || {100} $SrTiO_3$ orientation relationship and develop the understanding of the process at the atomic level. To be able to exert control over the nucleation crystallization process the interplay between interfacial free energy and supersaturation was investigated. For that purpose, we determined the lattice mismatch between {110} plane in $Bi_4Ti_3O_{12}$ and {100} in $SrTiO_3$. The misfit was found to be 1.78 %, which is an unavoidable contribution to interfacial free energy. On the contrary, our results accord with the theory and we can influence the nucleation and growth of $SrTiO_3$ by supersaturation and therefore, control the process by changing the molarity of NaOH and the initial Sr:Ti molar ratios. For example, at conditions with the initial stoichiometric Sr:Ti molar ratio and lower (2M) NaOH concentration the supersaturation is not large enough to enable $SrTiO_3$ overgrowth over the whole $Bi_4Ti_3O_{12}$ basal surface planes. Instead, $SrTiO_3$ island growth prevails. As the supersaturation increases by increasing the initial Sr:Ti molar ratio, the number of $SrTiO_3$ nuclei is becoming larger and their size is becoming smaller. Finally, at a 12-times higher Sr:Ti initial molar ratio than needed for theoretical $SrTiO_3$ formation, the layer-by-layer growth mechanism prevails over the island formation mechanism causing the intermediate $SrTiO_3/Bi_4Ti_3O_{12}$ and final $SrTiO_3$ nanostructures retain the platelet shape of the template. Understanding this particular transformation mechanism provides general design principles for the preparation of two-dimensional nanoheterostructures with epitaxial contact.

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Strontium Hexaferrite Magnets Sintered by Intense Thermal Radiation (SITR)

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Multitude of modern technologies rely on permanent magnets for their operation. Despite the overwhelming superiority in performance of magnets based on rare-earth elements the harmful environmental impact of their production, uneven distribution and increasingly questionable supply due to geopolitical fluctuations force us to look for alternatives. One such solution emerges from the group of hexagonal ferrites [1]. M-type ferrite magnets generally do not contain critical raw materials [2]. Ba and Sr hexaferrites are in terms of volume one of the most used permanent magnetic materials in the world [3].

In our study we investigated Sintering by Intense Thermal Radiation (SITR) of strontium hexaferrite. Although this material and the sintering process have been known for some time, up till now this approach was not used to consolidate this widely used magnetic material. Sintering was performed in an SPS device with a modified graphite model that enabled isolated radiation sintering. The research focused on the correlation between the processing parameters and the magnetic properties of produced material. Several parameters were tested, among which the sintering temperature and the magnetic orientation of the particles before compression had a positive effect on the magnetic properties. Some of the parameters we tested did not show an effect, but some had a markedly negative effect on the magnetic properties of sintered samples. The best combination of parameters at the moment are: a magnetically non-oriented sample, which is uniaxially compressed in a floating matrix heated to a sintering temperature of 1100 ° C at a speed of 500 K / min and kept at this temperature for 5 minutes.

The sample prepared in such a way displayed promising magnetic properties, especially in terms of coercivity. (H_C=344.4 kAm, M_r=44.9 Am^2kg^{-1}, M_S=65.9 Am^2kg^{-1})

Key words: Strontium hexaferrite, magnets, magnetic properties, sintering, SITR

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Synthesis and crystal structures of $a XeF_2 \cdot b MnF_4$ compounds

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During the study of the catalytic impact of MnF_3 on the reaction between Xe and F_2, it was observed that a solid phase with composition $XeMnF_x$, where x varies between 5 and 6, forms [1]. Subsequent studies identified this compound as $XeF_2 \cdot MnF_4$ and revealed the presence of two other adducts in the XeF_2–MnF_4 system, namely $3XeF_2 \cdot 2MnF_4$ and $XeF_2 \cdot 2MnF_4$ [1, 2, 3]. The crystal structure determination of the compounds belonging to the XeF_2–MnF_4 family was highly sought after, as they could be structurally related to their platinum analogues and thus to the first noble-gas compound "$XePtF_6$", the exact chemical nature of which is still unknown [4]. In the present study, we redetermined the crystal structures of $3XeF_2 \cdot 2MnF_4$ and $XeF_2 \cdot MnF_4$ with improved figures of merit in comparison to the original report [3] and determined the crystal structure of $XeF_2 \cdot 2MnF_4$ for the first time. Action of excess molten XeF_2 on MnF_2 in a nickel autoclave at 120 °C afforded $3XeF_2 \cdot 2MnF_4$, which upon solvolysis in anhydrous HF and removal of excess XeF_2 yielded $XeF_2 \cdot MnF_4$. Single crystals of $XeF_2 \cdot 2MnF_4$ were prepared by heating a mixture of XeF_2 and MnF_4 in a molar ratio of 1:2 in a sealed FEP ampoule at 120 °C. The compounds were characterised by single-crystal and powder X-ray diffraction and Raman spectroscopy. The extent of XeF_2 ionization [5] in studied compounds is also discussed.

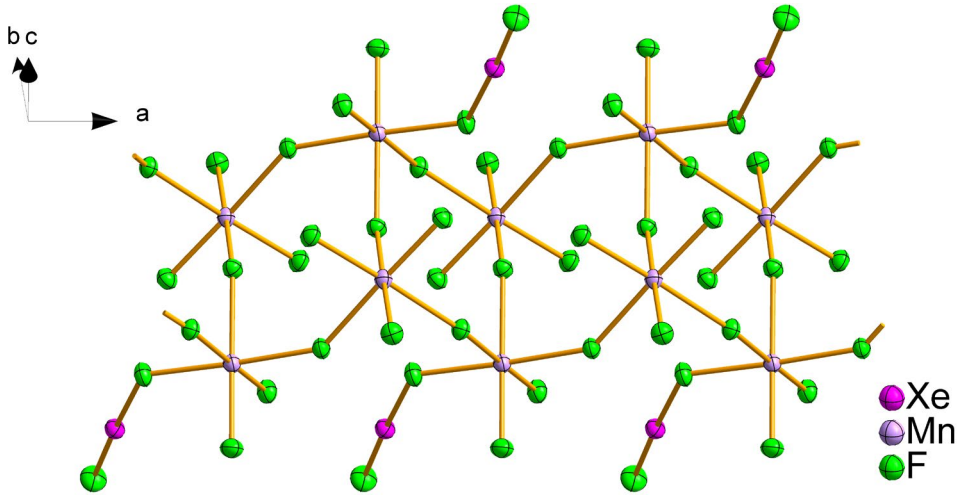

Figure 1. Crystal structure of $XeF_2 \cdot 2MnF_4$ (thermal ellipsoids are drawn at the 50% probability level)

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Synthesis of ceria catalyst support for magnetically heated catalysis

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Many important chemicals and fuels are industrially produced with catalytic reactions. To achieve significant rates of the reactions on catalyst increased temperature is required. Magnetic heating is an energetically-efficient way to provide the heat needed for catalytic reactions. The heat is produced by magnetic catalyst exposed to an alternating (AC) magnetic field of high frequency (several hundreds of kHz). The magnetic catalyst is a nanocomposite material containing magnetic nanoparticles dispersed in a catalyst-support matrix with a high specific surface area. Catalytic nanoparticles, e.g., Ru nanoparticles, are deposited on the surfaces of magnetic-nanoparticles-containing catalyst support. When exposed to an AC magnetic field the magnetic nanoparticles heat-up due to the hysteresis or relaxation losses. The selective and local heating of catalyst surface can enhance catalyst activity and energy efficiency of the catalytic process [1]. Since almost all noble metals and metal oxides used as catalyst nanoparticles are relatively thermally unstable and additionally have a very low surface area due to sintering, they are usually deposited on a support that keeps the active particles unisized and dispersed. Selecting the proper catalyst support depends on several criteria, such as particle size, morphology, surface area, porosity, chemical properties (acidity and basicity, hydrophobicity and hydrophilicity) and/or catalyst nanoparticle–support interaction. Catalyst supports are usually inert and refractory, most commonly used are carbon, alumina (Al_2O_3), and zirconia (ZrO_2).
In this work, ceria (CeO_2) was used as the support material of magnetic catalyst [2]. The catalytic particles were synthesized with deposition of the ceria onto citric-acid-coated maghemite (γ-Fe_2O_3) nanoparticles using the controlled precipitation of Ce ions in the aqueous suspension. The aim was to enable a heterogeneous nucleation of the precipitating Ce ions on the surfaces of the maghemite nanoparticles. To enable the required close control of the supersaturation during the precipitation the Ce^{3+} ions were immobilised with hexamethylenetetramine (HMTA) into a coordination compound. The controlled release of the reactive Ce^{3+} ions was enabled with slow thermal decomposition of the coordination compound. The synthesized composite particles were characterized with a combination of transmission electron microscopy and X-ray diffractometry. The results show that the ceria is formed in complex and multistep reactions.

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Tailoring the microstructure of $Li_{0.33}La_{0.56}\square_{0.11}TiO_3$ through exaggerated grain growth

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Increasing demand for energy requires safe, stable, and powerful energy storage. One of the promising solutions are rechargeable Li-ion batteries with solid electrolyte and in particular perovskites such as $Li_{0.33}La_{0.56}\square_{0.11}TiO_3$ (LLTO) with excellent ionic conductivity [1], [2]. While LLTO grains may reach ionic conductivities as high as 10^{-3} S/cm, the grain boundaries exhibit orders of magnitude lower values that decrease the total ionic conductivity of the electrolyte. Our strategy to reduce the contribution of grain boundaries was to prepare coarse-grained LLTO by triggering exaggerated grain growth of LLTO grains, as previously reported in several other perovskite-based systems [3]. The samples with La:Ti ratios from 0.56 to 0.62 by systematically lowering the addition of TiO_2 were prepared via a conventional solid-state approach and sintered at 1250 and 1350 °C. The stoichiometric sample shows a typical uniform microstructure with an average grain size of ~5 μm, whereas the sample with La:Ti ratio of 0.61 has bimodal grain size distribution composed of elongated grains measuring up to 100 μm in length and surrounded by smaller grains. In this sample, we observed the presence of polytypic lamellae with structural characteristics of Ruddlesden-Popper type $Li_2La_2Ti_3O_{10}$ phase and the elongation of the grains in the direction of the lamella. The presence of polytypic lamellae accelerates the growth of the matrix LLTO grains in the initial stages of grain growth (up to 1250 °C). The lamellae are thermally unstable at higher sintering temperatures (1350 °C) and recrystallize to perovskite LLTO. The result is LLTO ceramic microstructure with extremely large grains, measuring even more than 100 microns in diameter. To our best knowledge, a microstructure with so large grains has not been reported in LLTO ceramics before.

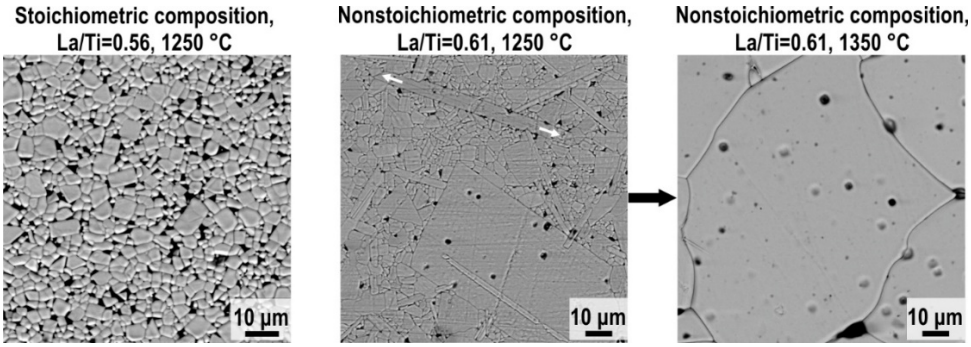

Figure 1. LLTO microstructure at different sintering temperatures and La/Ti ratio.

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Thin-film lithium manganese oxide cathodes synthesized by pulsed laser deposition

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Thin-film lithium-ion batteries have shown great potential for investigating properties of the intrinsic material and pursuing development of solid-state batteries. In order to study intrinsic properties of the material, additive-free cathodes are synthesized with pulsed laser deposition technique. One of the promising materials to use as a thin-film cathode is lithium-rich manganese oxide Li_2MnO_3 (LMO), due to its high specific capacity of 458 mAh/g. Nevertheless, the mechanism of lithium intercalation/deintercalation for Li_2MnO_3 is not fully understood; it has been reported that is intrinsically inactive because of high valence state of Mn^{4+}, still nanosized LMO is activated upon initial cycle and appears to have high specific capacity [1]. Significant amount of work was done on LMO thin-films, prepared with pulsed laser deposition technique, where the influence of deposition parameters on structure, morphology and electrochemical properties is thoroughly studied. In order to achieve high-quality thin-films with desired composition and crystal structure, one should carefully control an amount of lighter elements that can be scattered during plasma expansion, so thin-films of LMO often result in lithium and oxygen deficiency. To challenge this problems, lithium enriched targets are used to synthesize stoichiometric thin-film [2]. The aim of our research is understanding the influence of experimental parameters on final properties of synthesized thin films. In our work we synthesized LMO thin-films from home-made target with composition $Li_{3,2}MnO_3$ (60% lithium excess) on single crystal 0,5%wt Nb-doped $SrTiO_3$ (Nb:STO) substrates with (001) and (111) crystal orientation. We analysed synthesized thin-films using XRD to study the influence of Nb:STO substrate orientation on thin-film growth direction and AFM to determine morphological properties of the film.

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Tungsten–copper composites as advanced heat sink materials for fusion application

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Divertor is a vital component of the fusion device, designed to extract heat and plasma impurities and to protect the surrounding walls from thermal and neutron loads. Therefore, it is subject to the highest heat loads in the reactor. According to the current design, the DEMO divertor consists of serial array of rectangular units, tungsten monoblocks, connected to a copper alloy (CuCrZr) cooling tube running through the central region of the monoblocks. Tungsten serves as a functional plasma-facing armour material, whereas, the copper alloy tube acts as a structural heat sink to remove the heat from the first wall. Maintenance of structural integrity under high-heat-flux (HHF) fatigue loads is a critical concern for assuring the reliable HHF performance of a plasma-facing divertor target component. Next to the failure of plasma facing W due to plastic low cycle fatigue (LCF) cracks, failure at the W-Cu interface as a result of stress accumulation and/or neutron embrittlement of the Cu interphase is a major concern.

To mitigate this risk of interphase failure, a functionally graded transition between the heat sink and the armour material is proposed. W lattice structures were manufactured using field assisted sintering technique (FAST) followed by infiltration of Cu melt into a porous preforms, resulting in a W-Cu composite material. A series of W samples with variation in porosity was produced by variation of initial W particle size. During molten Cu infiltration the effects of temperature and atmosphere on the infiltration process were evaluated. Final W-Cu composites were characterised in terms of density and microstructure.

Using ATAC-seq to study chromatin level regulation of response to stress in potato

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Potato is the most widely grown tuber crop in the world and its demand is increasing due to global population growth. Climate change, accompanied by heat, drought, and floods, poses a major risk to crop production [1], thus innovative crop production strategies are urgently needed. Recent advances in genomics are enabling the rapid identification of genes related to stress resistance to breed crops adapted to the changing climate [2]. One such advance is the genome-wide identification of chromatin accessibility using transposase-accessible chromatin with high-throughput sequencing (ATAC-seq), which allows us to identify accessible chromatin regions (ACRs) involved in stress response regulation [3]. Little is known of chromatin accessibility in plants and even less so in potato, where ATAC-seq have not yet been used.

As part of my PhD work, we will expose potato plants to heat, drought, flooding and combinations of these stressors. We will sample potato leaves use ATAC-seq to identify ACRs. Applying ATAC-seq to plants is challenging because of organelle genome contamination [3] therefore optimization of plant nuclei isolation will be needed. Contamination of ATAC-seq library with mitochondrial, plastid and de-chromatinazed DNA will be estimated with quantitative PCR assays. We will design test and validate two sets of primers: first targeting conserved mitochondrial and plastid sequences and second targeting known known accessible and inaccessible regions of potato genome. After quality control, ATAC-seq library will be sent to short-read Illumina sequencing.

Sequenced reads will be subjected to bioinformatic analysis to identify ACRs in potato genome. We will build a computational pipeline consisting of: 1) quality control of reads including trimming of sequencing adaptors, deduplication and filtering of low quality reads; 2) alignment of cleaned reads to potato genome; 3) peak-calling of ACRs; 4) peak differential analysis and 5) motif enrichment. Combining our new data on accessibility with existing data on gene expression, transcription factors and transcription factors motifs will provide a holistic view on regulation of stress response in potato and aid exploration of targets for resilience breeding.

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Using Response Surface Methodology to optimize a zirconium conversion coating

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In a conversion coating (CC), the surface of a metal is converted via chemical reaction into an adherent and insoluble layer of more corrosion-resistant material. As such, CCs are often found as the primers providing anti-corrosion and adhesion promoting properties in the aircraft and automotive industry [1], where environmentally and budget-friendly zirconium conversion coatings based on hexafluorozirconic acid (H_2ZrF_6) gained significant attention during the last decade. In this work, the deposition process of zirconium conversion coating on cold-rolled steel (CRS) was optimized to achieve the best corrosion protection of CRS. The following bath parameters (pH, immersion time and H_2ZrF_6 concentration) were optimized regarding corrosion properties via Response Surface Methodology (RSM), where a mathematical model of the system is created from experiments performed according to statistically selected sets of variable combinations [2]. Central Composite Design (CCD) was employed by varying each input parameter on five levels: pH (3.0, 3.4, 4.0, 4.6 and 5.0), immersion time (60, 230, 480, 730 and 900 s) and H_2ZrF_6 concentration (150, 424, 825, 1226 and 1500 ppm). Polarization resistance (R_p), as an indicator of corrosion protection of CRS, measured by Electrochemical Impedance Spectroscopy (EIS) in a diluted Harrison solution, was chosen as a response. The obtained RSM plots (Figure 1) show both individual and mutual influences of the variables on the resulting response, from which optimum conditions can be easily predicted and tested [2]. The results show that the most influential parameter on the final coating quality is pH and that high values of R_p can be obtained at lower input parameter values, thus improving the process quality. Moreover, RSM can help to accelerate the overall coating development and shed a light on the further research in the chemistry behind it once the main parameters and their interactions are known. This knowledge can be extended further to formulate individual baths with more additives to obtain the desired performance.

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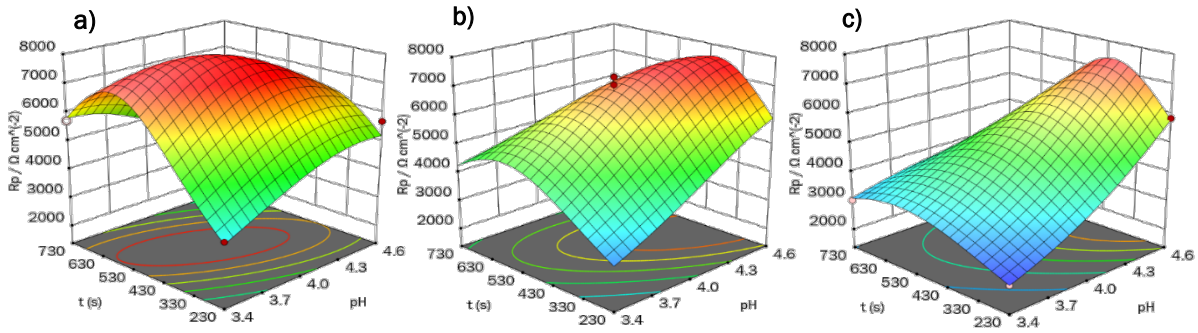

Figure 1. RSM plots of R_p on CRS at different H_2ZrF_6 concentrations: a) 424 ppm, b) 825 ppm and c) 1226 ppm.

Senzorske tehnologije
(Sensor technologies)

Creating antimicrobial surfaces via advanced functionalization techniques

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Microbes are all around us, in the air that we breathe, in the food and water that we consume, and on surfaces which we encounter. Although we've learned to co-exist and in some cases even harness their power (e.g., fermentation), some of them are still problematic, by causing disease or spoiling resources. Touching or using pathogen-laden items, such as tools, textiles, electronics and the like, can transfer them to susceptible surfaces, where they can propagate uncontrollably, expel harmful substances and present a new source for further spread. Using an advanced functionalization technique, we've developed a modified surface, which can disrupt microbial function, once it touches said surface. We were able to produce an activated surface, which can then serve as a carrier for an antimicrobial substance or material. To demonstrate this ability, we've chosen a surface-active agent. The surface treated with advanced functionalization technique was saturated with a solution containing the active substance, let to dry, and subsequently contacted with an infectious organism. The prepared material was able to reduce the number of microbes present by over 7 $\log_{10}$ units in 2 hours, verified by a plaque assay. What is more, reducing the amount od substance on the treated material resulted in a reduced antimicrobial activity, while the activated material alone caused insignificant reduction, demonstrating the effect is dependent on the amount of active ingredient. Large surface free energy of the chosen polymer prohibits the active substance to be efficiently applied, thus making the functionalization technique a prerequisite for an efficient application of said substance. This approach may lead to creating functional materials, which can be applied in all industries and areas where unwanted microbes can cause harm, for example medical, food, agriculture or water treatment sectors.

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Influence of Solution Formulation on Microstructural Features of Solution-Derived Barium Titanate-Based Thin Films

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Lead-free piezoelectric ceramics based on $0.5Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.5(Ba_{0.7}Ca_{0.3})TiO_3$ (BZT-BCT) are a potential replacement for commercially most wide-spread piezoelectric ceramics based on $(Pb(Zr,Ti)O_3$ or PZT) [**Error! Reference source not found.**], especially in room-temperature piezoelectric applications. For the design of devices, especially micro-electro-mechanical devices (MEMS), the materials in the thin-film form are used. Certain parameters such as grain size and shape, phase purity, and chemical homogeneity that influence the functional properties of thin films are controlled in the Chemical Solution Deposition (CSD) of barium titanate ($BaTiO_3$, BT) thin films [2]. The latter can be considered as a reference for BZT-BCT thin films.

Alkaline-earth acetates and transition metal alkoxides are the usual reagents in CSD of BT-based thin films processing. Carboxylic acids and alcohols are the most often used solvents to dissolve and dilute respectively alkaline-earth acetates and transition metal alkoxides [1]. BZT-BCT coating solution prepared following the conventional procedure for thin-film processing by CSD which includes carboxylic acid and ether-alcohol solvents was stable for about 2 weeks. We modified the coating solution preparation method shown in Figure by using ethylene glycol (EG) instead of carboxylic acid to dissolve the acetates. Thus, the stability of the BZT-BCT coating solution was increased from weeks to months. The coating solutions of both BT and BZT-BCT prepared by the combinations of EG and ethanol (EtOH), or EG and 2-methoxyethanol (2-MOE) are stable up to a least 2 months. The crystallization process and microstructural features of BT and BZT-BCT films prepared from solutions with different solvent mixtures are discussed in this contribution, as well as their dielectric, ferroelectric, and local piezoelectric properties.

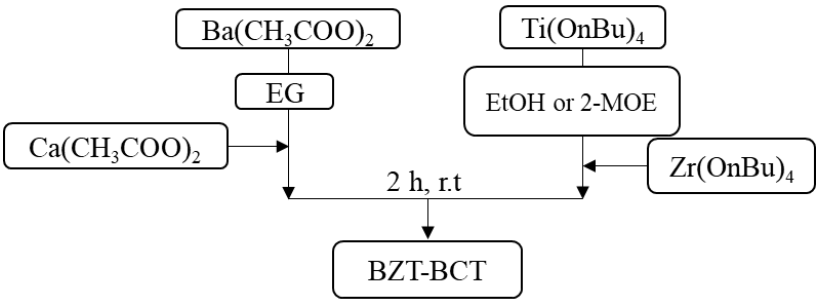

Figure 1. Synthesis of BZT-BCT coating solutions

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Integration of relaxor-ferroelectric 0.9Pb($Mg_{1/3}Nb_{2/3}$)O_3–0.1$PbTiO_3$ thick films on polymer substrates

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To miniaturize functional devices, electroceramic components need to be scaled down to micrometer level. The aerosol deposition (AD) method offers a cost-efficient way to deposit dense, micrometer-thick films at room temperature enabling the integration of ceramic components onto various substrates such as metals and polymers [1], [2]. In this context, relaxor-ferroelectric (1-*x*)Pb($Mg_{1/3}Nb_{2/3}$)O_3–*x*$PbTiO_3$ (PMN–100*x*PT) ceramic materials show excellent electro-mechanical properties, energy storage and energy conversion capabilities, suitable for electric generators, capacitors and electrocaloric refrigerators.

In this work, a few micrometer-thick PMN–10PT films were deposited by the AD method on flexible polyimide substrates. Reports show that compressive stresses generated in the thick films during the AD process relax after thermal annealing at 300–500 °C [3], [4]. PMN–10PT thick films thermally annealed at 400 °C attain a relaxor-like polarization vs. electric field hysteresis loops with high maximum polarization (above 38 $\mu C \cdot cm^{-2}$) and a very high dielectric breakdown strength (~1000 $kV \cdot cm^{-1}$), which makes them promising for energy storage applications. The total recoverable energy density of PMN–10PT thick films reaches ~10 $J \cdot cm^{-3}$ at ~1000 $kV \cdot cm^{-1}$. Moreover, the energy storage properties of PMN–10PT on flexible polyimide substrates are very stable after 10^5 bending cycles (at 1.0% bending strain). The importance of the AD method in the integration of ceramic thick films on affordable flexible polymer substrates will be discussed in this contribution.

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Optimization of materials on a working electrode for the determination of neonicotinoids

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Neonicotinoids are systemic pesticides with selective activity on acetylcholine receptors of insects. Because of their low toxicity for vertebrates, their use in the years following the initial commercialization has grown exponentially. In the last decade, they have been a target of many critics for their toxicity against pollinators, such as bees, which is the main reason for the extensive research in the field of analytical method development. These methods are mostly based on separation techniques such as high pressure liquid chromatography coupled to diode array detector or tandem mass spectrometry. Due to additional problems these methods bring, including long procedure time, large amounts of solvents and consequently higher price, a lot of recent research has been focused on fast and selective electrochemical sensor development.

The aim of the research was optimization and testing of different materials, used as a modification on the working electrode for the determination of three neonicotinoids.

Firstly, the quantity of reduced graphene oxide (rGO) in respect to nafion and metal oxide microparticles was optimized by preparing dispersions with different ratios of materials, previously prepared in a mixture of ethanol and ultrapure water (1:1). Commercially available screen printed carbon electrode's (SPCE) surface was modified with two layers of prepared dispersions by »drop-casting« method. Cyclic voltammetry (CV) was applied to scan 1 mM solutions of imidacloprid, thiamethoxam and clothianidin, with 12 % acetonitrile (ACN) in 0.1 M phosphate buffer solution (PBS) at approximately neutral conditions used as media. Optimal response was achieved at the volume ratio rGO (1 mg/mL) : metal oxide (1 mg/mL) : 5 % nafion being 6 : 3 : 1. Similarly, suspensions of forementioned materials were prepared at higher concentrations and SPCE was modified in the optimized ratio as described previously. It was concluded that highly concentrated dispersions do not significantly improve current response and will therefore not be used in further research.

Using suspensions of six types of metal oxide microparticles (Co_3O_4, MnO_2, Mn_2O_3, Fe_2O_3, Bi_2O_3 and RuO_2), two types of metal nanoparticles (W and Mo), rGO and 5 % nafion, different dispersions at previously optimized ratio were prepared and drop-casted onto SPCE. Similarly, a blank electrode was prepared with the main purpose to study a response on modified electrodes relative to the blank electrode. It was shown that Co_3O_4 significantly decreases the current peaks for all analytes, whereas the greatest enhancement was achieved by adding MnO_2 and Mn_2O_3 microparticles or Mo nanoparticles. However, the peak potentials as determined by CV were still too similar to achieve the desired selectivity. Cyclic voltammograms for every analyte were also measured at different scan rates of 20-200 mV/s. It was shown that the process is diffusion controlled.

Future work will be focused on optimizing the deposit modification, while using smaller sized particles with the aim of achieving better selectivity among tested insecticides and higher current response relative to background.

Predicting deep body temperature (Tb) from forehead skin temperature: Tb or not Tb?

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The Severe Acute Respiratory Syndrome Coronavirus-2 pandemic has identified the need to accurately screen individuals for signs of fever using skin temperature (T_{sk}), which may also aid thermally stressed workers, particularly during summer heatwaves (HW), to screen for heat strain. This study assessed whether T_{sk} measured at the forehead and fingertip could serve as an accurate and valid index of deep body temperature (T_b) during a simulated 3-day heatwave, and whether measurement of multiple sites could improve this prediction. Seven participants maintained a schedule of work, rest, and sleep over nine consecutive days split into three 3-day parts; thermoneutral pre-HW (25.4°C), simulated HW (35.4°C), thermoneutral post-HW. Continuously each day, contact thermistors measured forehead ($T_{forehead}$), and fingertip (T_{finger}) T_{sk}, and gastrointestinal temperature (T_{gi}) with a radio pill. Additionally, proximal-distal temperature gradient between forehead and fingertip ($\Delta T_{forehead\text{-}finger}$) was measured. Measurements were grouped into ambient conditions: 22, 25, and 35°C. T_{gi} and $T_{forehead}$ only displayed a significant relationship in 22°C (r: 0.591; p<0.001) and 25°C (r: 0.408; p<0.001) conditions. A linear regression of all conditions identified $T_{forehead}$ and $\Delta T_{forehead\text{-}finger}$ as significant predictors of T_{gi} (r^2: 0.588; F: 125.771; p<0.001), producing a root mean square error of 0.26°C. Additional residual analysis identified $T_{forehead}$ to be responsible for a plateau in T_{gi} prediction above 37°C. Contact $T_{forehead}$ was shown to be a statistically suitable indicator of T_{gi} in non-HW conditions, however an error of ~1°C makes this physiologically redundant. Measurement of multiple sites may improve T_b prediction, though it is still physiologically unsuitable, especially at higher ambient temperature.

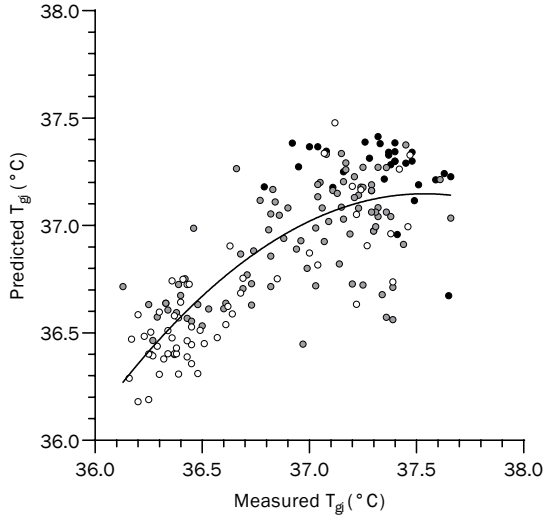

Figure 1. Relationship between measured temperature of the gastrointestinal tract (T_{gi}) and predicted T_{gi} using equation 1. Measurements and predictions based on skin temperatures were obtained while participants were exposed to three ambient temperatures: 22 °C (white dots), 25 °C (grey dots), and 35 °C (black dots). A second order polynomial trendline (y = -0.4464x2 + 33.512x - 591.75) represents the best fit (r2 = 0.63).

Preparation and Electrochemical Characterization of Screen-Printed Graphite Electrodes

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Screen printing technology is widely used to fabricate electrodes for electrochemical sensors, which have gained popularity in recent decades [1]. Apart from the low cost and the possibility of mass production, screen-printed electrodes also have the advantage of ensuring a reasonable level of reproducibility, miniaturization, and on-site analysis. Due to their low electrical resistance, stable chemical properties and wide potential window, carbon materials are widely used as working electrodes for the detection of pollutants, small biomolecules, food additives and heavy metal ions [2]. The aim of this work was to prepare a working electrode based on commercial graphite powder for the detection of neonicotinoid pesticides. The prepared layers should have a homogeneous and conductive surface, good adhesion to the ceramic substrate and a reproducible electrochemical response for the analyte(s) of interest.

Graphite paste with a solid content of 15 vol% was prepared by dispersing graphite powder in terpineol with cellulose. The paste was then screen printed through an 8mm x 8mm square mask onto an alumina substrate. Thermogravimetric analysis showed that the graphite powder did not decompose in an argon atmosphere up to 900 °C. Therefore, the layer was annealed at 450 °C and 850 °C, resulting in homogeneous, 50-60 μm thick graphite electrode (GE) with sheet resistivity of 55 and 5 Ω/sq, respectively. The sheet resistance was determined with 4 probe measurements. The poor adhesion of graphite to alumina surface was improved by adding glass to the graphite. A paste with a solid content of 15 vol% was prepared by mixing 75 wt% graphite and 25 wt% glass powder. The screen-printed graphite-glass layer annealed at 850 °C (GGE) was homogeneous, 40-50 μm thick and had a sheet resistance of 7 Ω/sq. The electrochemical response of GE and GGE was studied by cyclic voltammetry in a phosphate buffer (pH=7) solution using an equimolar concentration of potassium hexacyanoferrate(II)/(III). Commercially available Ag/AgCl reference and platinum sheet counter electrodes were used. Electrochemical measurements showed that the GGE has a capacitive current around 0.3 mA, a potential window of at least -1.6 to 1.0 V in the presence of only the supporting electrolyte. A peak-to-peak potential separation of approx. 140 mV and ratio of cathodic to anodic peak current above 0,95 were determined for measurements of GGE in the presence of analyte.

Future work will be focused on modifying the GGE electrode with carbon nanomaterials and metal oxide nanoparticles to enable neonicotinoid pesticide detection.

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Sensors For Electrochemical Detection Of Benzenediols Using Modified-Screen Printed Electrodes

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Screen- Printed Electrodes modified with electrocatalysts (platinum on carbon, gold on carbon; 20% by weight) were used to achieve simple, compact, single-use sensor elements for the detection of benzenediols, Catechol (ortho), Resorcinol (meta) and Hydroquinone (para).

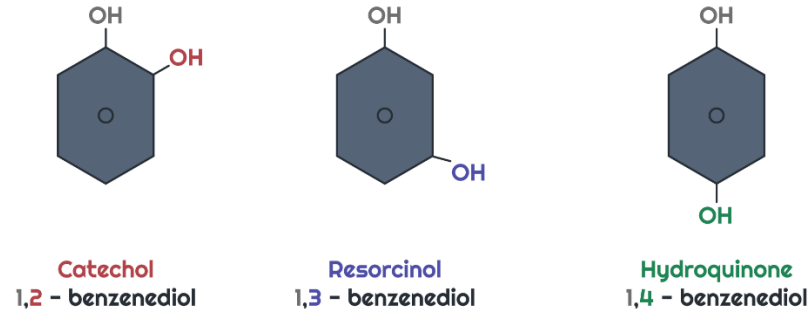

Figure 1: Structural description of benzenediols

Volatile Toxic Organic Compounds (VTOC) such as benzenediols were successfully detected on relatively inexpensive and accessible platforms such as Screen-Printed Electrodes. Through the use of carbon-supported catalysts, the desirable conditions required for excellent electrochemical activity i.e., large active surface area, high electrical conductance, which facilitates the detection of electrochemically active compounds, coupled with compact potentiostats show promise as a robust sensing instrument achieved due to relatively simple techniques such as cyclic voltammetry, chronoamperometry and differential pulse voltammetry which address the major requirements: selectivity, sensitivity, repeatability, linearity and portability. Calibration curves were recorded ranging from concentrations in the molar range down to the limit of measurements, 1 µM for catechol, 1 µM for hydroquinone and 100 nM for resorcinol. Although the detection was primarily facilitated by the use of high-performance catalysts, the simplicity of the electrodes holds the key to making the technology usable and accessible to potential everyday scenarios.

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Strategies for electrochemical genosensing of viruses and viroids

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Viruses are small infectious agents comprised of nucleic acids (DNA or RNA) covered by a protein coat, whereas viroids are small single-stranded circular RNAs without protein coating. Viruses can cause disease in humans, animals and plants, while viroids affect only flowering plants. The detection of viruses and viroids is typically achieved through conventional molecular biology techniques such as polymerase chain reaction (PCR) and enzyme-linked immunosorbent assay (ELISA). These techniques are gold-standard, with good limits of detection and precision, but they are laborious, time-consuming, and require specialised reagents and facilities. Electrochemical genosensors are a novel, straightforward option for detecting pathogens; they combine a biological recognition agent and a transducer to convert the molecular recognition event into a measurable signal. The construction of an electrochemical genosensor involves the modification of the electrode surface, the immobilisation of the biorecognition probe, and the following detection of the target gene sequence through DNA hybridisation. The amount of probe immobilised on the electrode surface should be optimised to allow for efficient hybridisation while maintaining the desired electrical properties of the transducer. Additionally, electrochemical genosensing can be improved by incorporating nanomaterials for signal enhancement or *in situ* amplification strategies to enhance their sensitivity and specificity.

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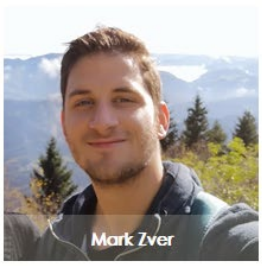

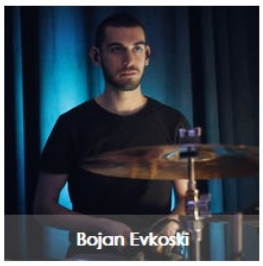

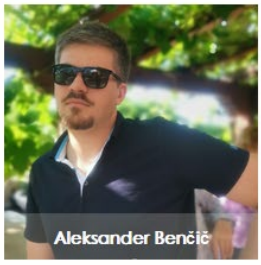


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