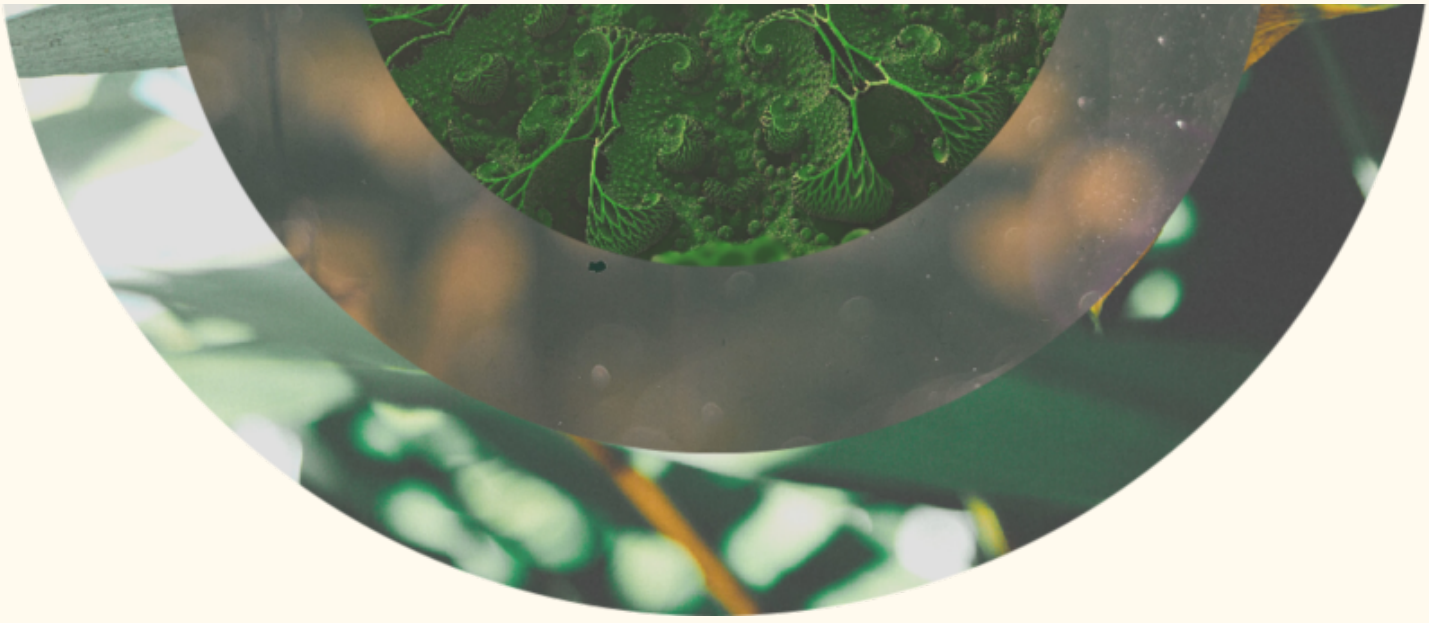
27 - 28 May 2021
Online

Institut
"Jožef Stefan"
Ljubljana, Slovenija

BOOK OF ABSTRACTS

Throughout knowledge towards a green new world



13TH STUDENTS' CONFERENCE OF THE JOŽEF STEFAN INTERNATIONAL POSTGRADUATE SCHOOL AND 15TH YOUNG RESEARCHERS' DAY OF CHEMISTRY, MATERIAL SCIENCE, BIOCHEMISTRY AND ENVIRONMENT

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13. ŠTUDENTSKA KONFERENCA MEDNARODNE PODIPLOMSKE ŠOLE JOŽEFA STEFANA IN 15. DAN MLADIH RAZISKOVALCEV (KONFERENCA KMBO)

Knjiga povzetkov

13th JOŽEF STEFAN INTERNATIONAL POSTGRADUATE SCHOOL STUDENTS' CONFERENCE AND 15th CMBE DAY

Book of abstracts

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Second Online IPSSC Conference – May 2021

Well, this was an interesting year, was it not? While physically removed from each other, we tried to compensate with digital tools, only to realize that it is not the same. How we miss all the meetings with our friends and colleagues, fun times in the office or the lab, networking at conferences and lectures. But let us not dwell on the negatives, but rather look at the opportunities these extraordinary circumstances have provided. We learned so much more about viruses and how they interact with humans and the environment, we saw how humanity reacts in a global crisis (including all the good and all the bad), and some days we were forced to disconnect from everything and just be bored for a while. Some people learned to bake bread, paint a sunset, play »Wonderwall« on guitar or just bought a new house plant and made their life a little greener. For all the bad and terrible, it is good to take stock and be thankful for all the bright spots.

This conference is now the 2nd online conference of the Jožef Stefan International Postgraduate School (IPS), combined with the Chemistry, Materials, Biochemistry and Environment (CMBE) Young Researchers' Day. Learning from last year, we tried to make the experience resemble an in-person conference as closely as possible, by providing digital rooms and 2D characters to move around with, speaker podiums, chairs and tables, board games and so much more. You were able to chat with each other, exchange ideas and your research work, network with potential employers or just play a round of Texas hold 'em with people you met for the first time. This is also a unique opportunity for students to mingle with professors, exchange ideas and make plans for collaborations. Some of you also took this opportunity to tick one of the most important boxes when stepping on the path to becoming a researcher – presenting your work to your peers.

So many excellent presentations and posters, such innovative perspectives, and research that has the potential to change the world. We think that organizing this conference is one of the most important tasks of the IPS Student Council. Even with all that is happening in the world, science must go on, scientific research and development cannot stop and wait, it is our duty to find a way to do our work and collaborate with others. While this online format is not an adequate substitute for the real thing, it is a way for us to give you a platform where you can share your work and continue improving yourself and your research. We are grateful to IPS for supporting this event, financially, and with all of the IPS staff that was always more than willing to help, also to all the IPS professors that contributed in numerous ways. Hats off to all of the sponsors that contributed so much this year, by financing our digital platform, filling up the goodie bags for all the participants, and even providing us with a financial boost for next year's conference, thank you! And we are thankful to all of you who attended this

conference, prepared your posters and presentations, and collaborated in so many other ways. Without you, there would be no conference.

"The reward of the young scientist is the emotional thrill of being the first person in the history of the world to see something or to understand something. Nothing can compare with that experience."

– Cecilia Payne-Gaposchkin

Enjoy the thrill!

The IPS Student Council and Organizing Committee of IPSSC

Beseda predsednika MPŠ: Akad. prof. dr. Vito Turk

Že več kot leto dni živimo in delamo v pogojih, ki jih v moderni dobi človeštvo še ni poznalo. To je čas pandemije, ki jo je povzročil novo odkriti in izjemno nevaren koronavirus (Covid-19), ki je razširjen po vseh kontinentih in državah. V svetu je prizadel že več kot 160 milijonov prebivalcev, umrlo pa jih je okoli 3.5 milijonov. Tudi naše države se Covid-19 ni izognil, saj je zbolelo okoli 250 tisoč naših državljanov in jih umrlo preko 4300. Izjemno breme je padlo na zdravstveno osebje, ki je z velikimi napori uspelo, da se je število obolenj pričelo zniževati. Hitro smo se morali prilagoditi novemu načinu vsakodnevnega življenja, kar terja veliko samodiscipline ter odgovornosti na vseh ravneh. Omejeni so bili in so še stiki med sorodniki, prijatelji, študijskimi kolegi in drugimi z namenom, da se širjenje pandemije upočasni in končno tudi ustavi, da bi lahko zopet normalno zaživeli.

Posledicam pandemije se tudi naša Mednarodna podiplomska šola Jožefa Stefana (MPŠ) ni mogla izogniti. Vse naše aktivnosti smo bili prisiljeni prilagoditi novim razmeram, kar je terjalo od vodstva šole, profesorjev in mentorjev ter naših podiplomcev popolnoma nov pristop k reševanju nastale situacije. Tudi seje študijskih komisij, senata in še bi lahko našteval smo morali izvesti s pomočjo internetnih komunikacij. Ob teh prilikah pa se je pokazalo, kako ključnega pomena je dobra organiziranost in sodelovanje na vseh ravneh delovanja naše šole. Tudi delo v raziskovalnih laboratorijih v teh izjemnih pogojih poteka kar uspešno, za kar gre zasluga tako magistrantom in doktorantom kot tudi njihovim mentorjem, ki delajo v raziskovalnih laboratorijih različnih institucij. Prepričan sem, da smo se v tem pogledu najbolje odrezali v Sloveniji, za kar gre vsem sodelujočim izjemna zahvala!

Danes je MPŠ uveljavljena podiplomska institucija v domačem in mednarodnem prostoru. 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 ter kakovostnimi mentorji. Prav tako je velikega pomena vključitev in sodelovanje Nacionalnega inštituta za biologijo (NIB) in Inštituta za kovinske materiale in tehnologije (IMT) v delovanje šole. Vse omenjeno pa daje poudarek interdisciplinarni naravnanosti ter vsestranskemu razumevanju sedanjega časa ob inovativnosti in odličnosti. Pojem »odličnost« se je v svetu uveljavil, še zlasti na področju znanosti. Pri različnih razpisih, še zlasti Horizon 2020, so uspešni le tisti projekti, ki dobijo oceno odlično ali celo izvrstno. Tudi nekaj naših raziskovalcev in profesorjev je med njimi. Žal pa pred dnevi objavljeni rezultati ERC projektov

odličnosti kažejo slabo sliko uspešnosti EU-13 držav, tudi Slovenije, kar je tudi posledica podcenjevanja financiranja znanosti s strani vlad. Rezultati osnovnih raziskav in osvojenih novih znanj vodijo s svojimi prelomnimi dosežki do novih inovacij in proizvodov, od katerih je odvisna ekonomska rast in moč države, tudi Slovenije. Na tem mestu naj poudarim, da to morajo razumeti tako politiki, ki vodijo državo, kot tudi gospodarstveniki. Zato pa je potrebnih 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 znanje! Kjer je znanje, pa so tudi investicije domačega in tujega kapitala in posledično novi proizvodi z visoko dodano vrednostjo. To dokazujejo uspehi razvitih držav in njihovih gospodarstev, ki ves čas povečujejo vlaganja v znanost in razvoj. Pri nas pa so med prvimi po pravilu na udaru znanost in raziskave, v končni posledici pa ceneni proizvodi z vsemi posledicami, kar to prinaša.

Izjemnega pomena je enakovredno mednarodno sodelovanje, kar pomeni, da le uspešni sodelujejo z uspešnimi oziroma razviti z razvitimi. V nasprotnem primeru najboljši iz manj razvitih držav odhajajo v razvite države, kjer doprinašajo k njihovi nadaljnji gospodarski in politični moči! To je beg možganov, ta čas največji, kar smo jim priča pri nas. Za Slovenijo velja, da bi morala vlada vlagati vsaj 1 % BDP, in to praktično takoj. Tako pa smo kljub že skoraj 10-letnim obljubam za dosego cilja 1 % trenutno pri okoli 0,4 % BDP ali prav pri dnu EU. Žal odgovorni vedno znova in znova dokazujejo, da vsega tega ne razumejo, kajti če bi razumeli, bi delali in ukrepali drugače.

Tudi letošnja predstavitev raziskovalnih dosežkov naših podiplomcev, kljub izrednim razmeram, je ponoven dokaz njihove uspešnosti. To je posledica trdega dela, talenta in veselja do pridobivanja odličnih novih znanj. Vse to vam omogoča, da se boste ob pomoči mentorjev ter bližnjih sodelavcev razvili v kreativne raziskovalce, na katere smo in bomo ponosni. S svojim znanjem boste lahko 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. Na potezi je vlada!

Ob koncu bi še enkrat ponovil, 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 doslej še nismo dočakali. Vendar bodimo optimisti, saj upanje umre zadnje!

Beseda dekanje MPŠ: Prof. dr. Milena Horvat (slo)

Čarobna beseda »znanje« se pogosto uporablja, vendar resnična narava te besede pride na dan, ko jo dokažemo z dejanji. Bogatenje znanja z delom in izkušnjami ima neizmerno moč, kar vodi k razvoju posameznika, skupin in družbe kot celote. Šola, v kateri študentje znanje pridobivajo z izkušnjami s konkretnimi dejanji, bo v življenju vsakega posameznika zagotovo zapisana z velikimi črkami. Na Mednarodni podiplomski šoli Jožefa Stefana (MPŠ) smo ponosni na delo študentskega sveta in vseh študentov. Študentje namreč svojo odločnost dokazujejo s konkretnimi dejanji – z znanjem in trdim delom pri doseganju pomembnih izzivov – in si tako utrjujejo karierno pot. Nič jim ni dano, ampak pridobljeno z njihovim odličnim delom. Pri tem ne smemo pozabiti na mentorje, ki učence usmerjajo in jim pomagajo doseči ambiciozne cilje – priznanje gre torej vsem, študentom, mentorjem, podpornemu osebju ter partnerjem in ustanoviteljem šole.

Tudi letošnja konferenca dokazuje, da so študentje seznanjeni z današnjimi izzivi in prednostnimi nalogami, zato ni presenetljivo, da je geslo konference »Skozi znanje k zelenemu novemu svetu«. Na to odločitev, zavzetost in odlično organizacijo smo zelo ponosni. Čestitke vsem – odgovornim za organizacijo in tistim, ki so se prijavili na konferenco!

Skupna organizacija dveh tradicionalnih študentskih konferenc – študentske konference MPŠ in dneva mladih raziskovalcev na področju kemije, materialov, biokemije in okolja (KMBO) na Inštitutu »Jožef Stefan« – se je izkazala za zelo učinkovito pri spodbujanju izmenjave znanja in izkušenj med študenti in raziskovalci. Ne glede na virtualno naravo konference je tudi letošnja konferenca posvečena praksam podajanja znanja na način, ki je razumljiv širokemu krogu ljudi.

Že lani so študentje dokazali, da znajo uporabljati sodobne pristope, ki omogočajo organizacijo virtualnih ali hibridnih konferenc, kar je omogočilo udeležbo večjega števila študentov. Trenutni omejevalni pogoji so tako povzročili priložnosti za prihodnost. Vsem udeležencem želim prijetno virtualno druženje in veliko uspeha pri nadaljnjem raziskovalnem delu.

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

The magic word "knowledge" is widely used, but the true nature of this word comes to light when it is demonstrated by actions. Enriching knowledge through and with experience has immense power, which leads to the development of an individual, groups and society as a whole. The school in which students gain knowledge through experience with concrete actions will certainly be written in capital letters in the life of each individual. At the Jožef Stefan International Postgraduate School, we are not only happy, but especially proud of the work of the Student Council and all students. This is because students prove their determination with concrete actions – through knowledge and hard work to achieve important challenges and thus pave their career path. Nothing is given to them but gained through their excellent work. In doing so, we must not forget the mentors who guide students and help them achieve ambitious goals – the acknowledgement therefore goes to all, students, mentors, support staff, and partners and founders of the school.

This year's conference also proves that students are familiar with the challenges and priorities of today, so it is not surprising that the motto of the conference is "Through knowledge towards a green new world". We are very proud of this decision, commitment and excellent organization. Congratulations to all – those in charge of the organization and those who registered for the conference!

Joint organization of two traditional student conferences – the IPS Student Conference and the Day of Young Researchers in Chemistry, Materials, Biochemistry, and Environment (CMBE) at the Jožef Stefan Institute – has proven to be very effective in promoting the exchange of knowledge and experience between students and researchers. Regardless of its virtual nature. This year's student conference continues with the previous year's practice of talking about science in a way that is comprehensible to a wide range of people.

Already last year, students proved that they know how to use modern approaches that allow the organization of virtual or hybrid conferences, which allowed the participation of a larger number of students. The current restrictive conditions have thus resulted in opportunities for the future. I wish all participants a pleasant virtual gathering and a lot of success in their further research work.

Prof. Dr. Ingrid Milošev (CMBE president)

Dear participants!

The Jožef Stefan International Postgraduate School Students' Conference (IPSSC) has merged with the Day of the Young Researchers of Chemistry, Materials, Biochemistry and Environment (CMBE) of the Jožef Stefan Institute. The main goal of the conference is to stimulate the discussion of the scientific results among students and facilitate the interaction between different fields. I am sure that this year's conference will maintain the tradition of previous conferences and establish a platform to present and communicate your newest results, to create personal contacts, to promote research and to find possibilities of cooperation. Young researchers are very valuable to us and deserve special attention. We wish you many new scientific ideas, but also friendly and relaxing gatherings with colleagues in the future. Although the conference will proceed online, we do hope that the friendly spirit of this conference combined with high scientific level will continue. We believe that it is highly important to maintain the enthusiastic spirit and other good traditions of the previous conferences.

Prof. Dr. Ingrid Milošev on behalf of the CMBE Commission of the Jožef Stefan Institute

Povzetki/Abstracts

Ekotehnologija (Ecotechnology)

An isotope perspective of urban water system

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Stable isotopes are important water fluxes tracers in urban areas and can identify water sources over different spatio-temporal scales. However, a considerable research gap is present in the understanding of water partitioning in those heterogeneous environments. Conducting the field studies across cities is challenging because monitoring of extensive spatio-temporal scales is needed to constrain different water fluxes, subsurface flow paths and high heterogeneity [1].

A systematic sampling of isotopes in precipitation, surface water and groundwater over the city landscape of Ljubljana, Slovenia was conducted to identify the changes in the spatio-temporal dynamics of water and were monthly collected at JSI-Reaktor, the Sava River at Brod and Šentjakob and from five wellfields (Kleče, Hrastje, Brest, Jarški prod and Šentvid). Overall, 12 monthly precipitation samples and snapshot samples of 22 surface water and 143 groundwater were analysed for the determination of oxygen ($\delta^{18}O$) and hydrogen ($\delta^{2}H$) isotope composition. Meteorological and hydrological data were also collected. Data collection focused on the year 2020 and results were compared to the data from the year 2010-2011 [2].

The isotope values of precipitation, river Sava and groundwater follow the general seasonality; more depleted in heavy isotopes in winter compared to the summer with more damped isotope values in surface water and groundwater. When comparing our results with data from 2010/11 it shows that the isotope composition changed; the average isotope composition of precipitation shows more positive values, while the isotope composition of surface water and groundwater more negative values. This can be attributed to the current trends of temperature increase and changes in water recharge. Due to the different method of investigation, a smaller scattering of data was observed. (Figure 1) [2].

Based on the results, we can demonstrate that water isotopes in urban areas have great potential for better comprehension of water partitioning in complex urban landscapes. The future work will include identifying the changes of the water fluxes with a focus on the contribution of river water versus local precipitation to the groundwater due to climate change.

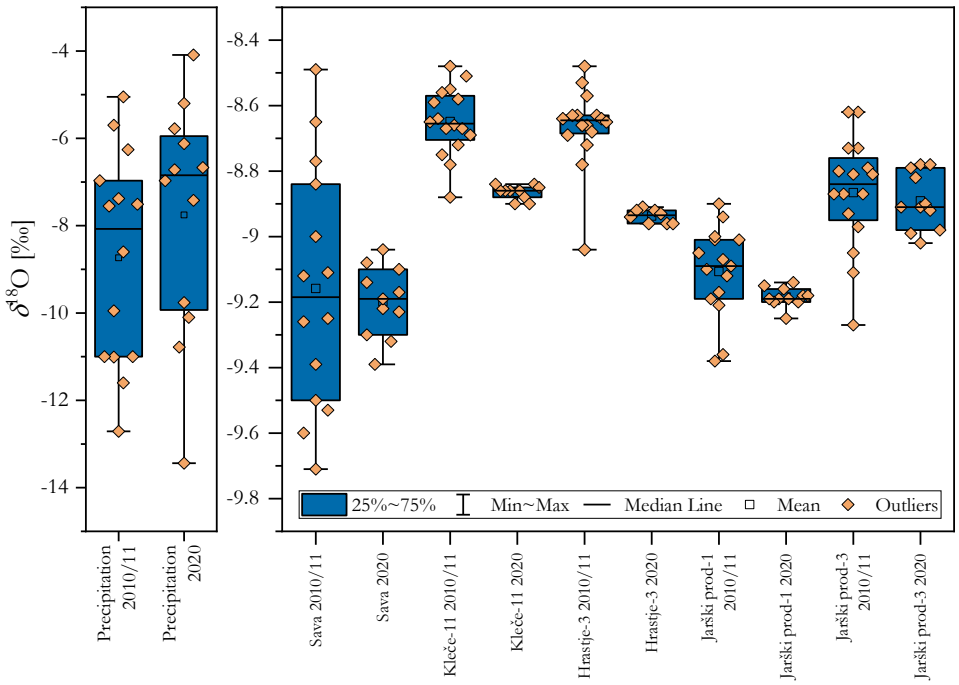

Figure 1. Variations of $\delta^{18}O$ values in precipitation, River Sava and groundwater for the period 2010–2011 and 2020.

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Funding: ARRS (Slovenian Young Researcher Program, Program P1-0143), IAEA CRP-33024 and IAEA RER-7013.

Bias in analytical methods: Bleomycin case study

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In analytical chemistry, the ability of a method to deliver accurate results is of great importance. But as a consequence of random and systematic errors, a difference, however small, between the measured and 'true' value is always present. Contrary to random error, systematic error or bias tends to remain constant or vary in a predictable manner when measuring under the same conditions. It should therefore be identified and corrected early on in the measurement process.

Assessment of bias requires a comparison of measurement results with a reference value, ideally established using certified reference materials (CRM), closely resembling real-life samples. Often, however, appropriate CRMs are not available in which case other methods of establishing reference values need to be resorted to. As a common alternative, surrogates (spikes) are used, which is less optimal as it introduces an additional step into sample preparation and is thereby an additional source of uncertainty.

To illustrate the importance of determining method bias, a case study is presented, evaluating and comparing different sample preparation methods for UHPLC-MS/MS quantification of bleomycin in plasma. The main goal of this research was to improve a formerly existent laborious and time-consuming sample preparation process. The newly developed shorter and simpler method would facilitate the preparation of larger batches of samples while still providing satisfactory clean-up and high recoveries.

Through the course of the development, three different methods for plasma sample clean-up were evaluated; 1) classical solid-phase extraction (SPE) on wide-polarity range sorbent Oasis HLB 96-well plates, 2) protein precipitation with acetonitrile, and 3) the combination of protein precipitation (0.1% formic acid in acetonitrile), with phospholipid removal using Ostro 96-well plates. The workflows for each procedure are presented in Figure 1. They were compared on the basis of their performance (matrix removal efficiency, recovery of the analyte, accuracy, repeatability) and overall complexity of the procedure.

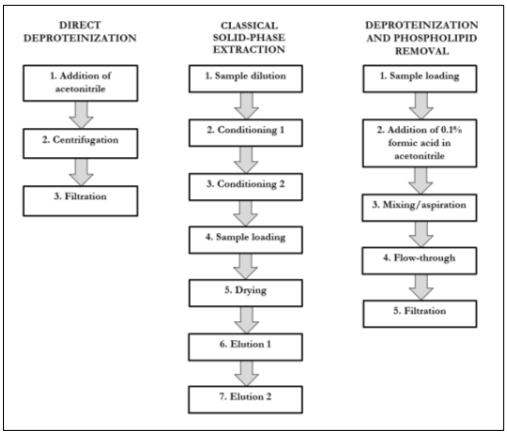

Figure 1. Workflows for sample preparation

Each of the three methods presents specific advantages and challenges. The advantage of the direct deproteinization method is its brevity and simplicity, though both classical SPE and phospholipid removal plates provide superior removal of matrix components, generating cleaner samples.

Apart from that, there are some noticeable differences among the final quantification results of individual methods, which are the consequence of method-dependent biases. Since no CRMs are available for bleomycin in plasma, and since there exist no candidate laboratories to compare our results with, these cannot be precisely defined and corrected. Nevertheless, measures can and should still be taken to minimize them. An efficient way to do so is to find suitable internal standards and to monitor the method performance through a longer period of time, which is going to be the next step in our research.

COVID-19 pandemic situation in Slovenia from the decision and risk analysis points of view

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Exposure to coronavirus (SARS-CoV-2) can lead to COVID-19 disease. Most of the infected only develop mild symptoms, while some get severely ill developing different complications that can result in death[1]. Risk analysis[2] aims to inform the decision-making about possibilities for reducing negative health effects. Evaluation of COVID-19 pandemic situation in Slovenia from the risk and decision analysis points of view aims to contribute to the clarification of COVID-19 related health risks, to identify areas requiring additional research and possibilities for improved mitigation of the pandemic impacts, and to shed light on the related decision-making process.

The formal management of the COVID-19 pandemic [3], [4] in Slovenia still lacks a clear identification of major concerns, priorities and determinants of decision-making (e.g. is it potential exposures, the number of infections, hospitalizations, deaths, etc. or all of these without specific prioritisation?). It is unclear how the publicly available information affect specific decision-making about mitigation measures. There are no clear follow-up evaluations of the purpose, implementation and effectiveness of specific mitigation measures. Social activities and personal behaviours potentially leading to SARS-CoV-2 exposure are major drivers of the COVID-19 pandemic, however, there is still a lack of data about the proportion of the exposed that were infected in specific exposure settings and situations. The communication of COVID-19 related risks is lacking in consistency, does not clearly address the public's perception of COVID-19 related risks and does not provide clear recommendations about what should people do, why, and how.

The observation of the situation as given above supports general media reporting that the level of public trust in the institutions responsible for the management of COVID-19 pandemic in Slovenia is continuously decreasing. Effective COVID-19 pandemic mitigation decisions require consideration of values of all relevant stakeholders in addition to various social, economic, legal, scientific, and political factors.

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Complex activity recognition using classification methods on low-cost portable ambient and activity sensor data

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Information is power, and equipping citizens with data about their living environment is fundamental in developing policies that reflect the needs and wants of the inhabitants of a specific space. Knowing what individuals are doing when they are exposed to elevated levels of pollution is crucial when implementing plans to reduce possible harm. Combining data from movement/heart rate sensors and environmental sensors can provide a large dataset with high temporal resolution. Utilising this dataset with machine learning methods can be used as a tool to recognize specific complex and simple activities that the individual is performing, without resorting to manual data logging. Research has shown promising results for recognizing simple activities, such as walking and running, but reliable complex activity recognition is still elusive [1], [2]. A wrist-worn smart activity tracker (measuring movement and heart rate) in combination with a wearable environment/ambient sensor (measuring particulate matter concentrations, temperature and humidity) were used with two groups of individuals who recoded specific activates they were performing through the day:

- group A recoded activities (e.g. "cooking", "cleaning", "running", etc.) with hourly resolution, as part of the ICARUS H2020 project [3],
- group B recorded with minute resolution.

The dataset from group A was modelled with three classification algorithms which are listed in **Table *1***, together with the results of correctly classified instances. Most misclassified instances were observed for activities with vague definitions, such as resting and playing, while more defined activities, such as smoking, cooking, cleaning and running had fewer misclassified instances. The accuracy could be improved by a clearer definition of activities, breaking more general ones into more specific and, crucially, increasing temporal resolution of activities from one hour to one minute. Preliminary results for group B showed improved results with accuracies >60%, though these results have to be further verified. This research provides a necessary first step of determining the usefulness of combining wearable ambient and activity sensors for complex activity recognition.

Table 1. Classifiers used and results of each model (for group A)

Classifier name	Classifier type	Correctly classified
IBk	k-Nearest Neighbors	32.7%
J48	decision tree	39.5%
Random Forest	random forest	43.1%

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Development and application of the method for determination of selected psychoactive pharmaceuticals in wastewater

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The psychological disorders causing anxiety, depression, insomnia and post-traumatic stress disorder reduce emotional stability. The burden of mental disorders is growing worldwide, leading to a significant impact on health and major social and economic consequences [1]. That is why the ability to monitor psychoactive pharmaceuticals use is of great importance. Conventional socio-epidemiological methods such as general population surveys, hospital records, prescription and sales data are typically used for monitoring pharmaceuticals [2]. These so-called traditional estimation methods have many limitations, and a need exists for an alternative approach. In this light, wastewater-based epidemiology (WBE) is one such innovative approach that can offer objective and complementary information about exposure to pharmaceuticals in defined population groups through the analysis of human metabolic excretion products (biomarkers) in wastewater [1]. WBE considers that excreted human biomarkers resulting from the consumption of pharmaceuticals are collected and pooled by the urban sewage system, providing valuable evidence in near real-time about the amount and type of substances used by a population (Figure 1).

This paper describes a method for determining 27 psychoactive pharmaceuticals (antidepressants, antipsychotics, benzodiazepines and Z-drugs) and their metabolites in wastewater. Analyte enrichment is achieved using solid-phase extraction (SPE), and the extracts are analysed using reversed-phase liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS). Accurate quantification is achieved by using deuterated standards. The developed method will be applied to municipal wastewater from five Slovenian and three Belgian wastewater treatment plants, differing in size, configuration and treatment strategies. Psychoactive pharmaceutical consumption will be estimated, while temporal and spatial trends will be evaluated and compared with socio-epidemiological studies.

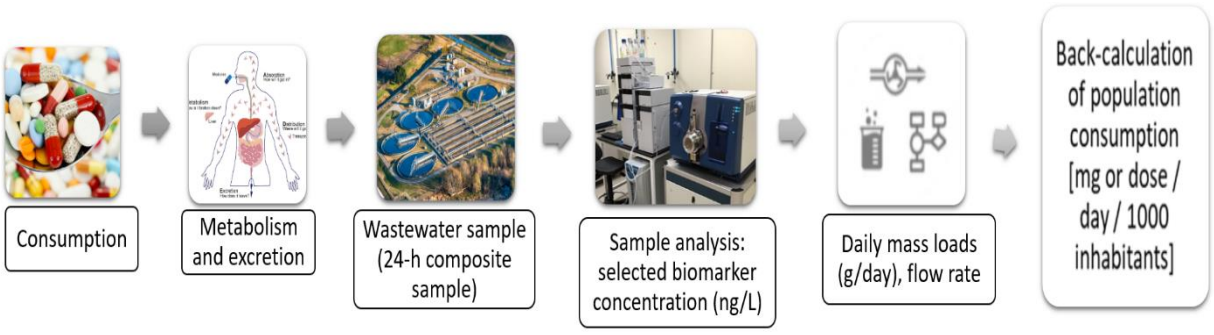

Figure 1. Scheme of WBE principle.

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Development of an analytical method for the determination of the isotopic composition of Pb in environmental samples

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Lead (Pb) is a naturally occurring element, that is one of the most toxic elements present in nature. That is why a lot of studies are focusing on measuring its concentrations in the environment [1]. In order to trace the sources of Pb, its isotope composition is determined [2]. Thermal ionisation mass spectrometry (TIMS) has traditionally been the method of choice for accurate and precise isotope ratio determination. Nowadays, multi-collector inductively coupled plasma mass spectrometer (MC-ICP-MS) is widely used. High precision isotope ratio determinations, regardless of the detection system, require quantitative isolation of the target element from its matrix prior to isotope ratio measurement. Commonly applied Pb separation methods involve the use of extraction chromatographic Pb spec resin, Sr spec resin and ion exchange resin such as Dowex 1X8. In order to achieve accurate and precise Pb isotopic composition, the Pb isolation from the matrix should be complete. This way we can assume no isotope fractionation occurred that would lead to biased interpretation of results.

The aim of this work was to compare the three resins in term of their efficiency in Pb isolation, possible Pb isotope fractionation, ease of use, and analysis time. For all three resins the isolation procedure in solid samples is as follows: microwave assisted digestion, pre-concentration, removal of matrix and Pb elution. For this purpose, Pb concentration and isotope composition were determined in different samples, namely in certified Pb isotopic standard (SRM 981), surface water, plant material, soil and outdoor-dust. The mass balance during the Pb isolation from the matrices was followed by measuring its concentration by ICP-MS. For the determination of Pb isotope composition MC-ICP-MS will be used.

So far, the results showed possible losses of Pb for all three resins during evaporation in a step for removal of the matrix (solution is an increased duration of the ultrasonic bath and an increased volume of acid for rinsing), during sample loading (molarity of acid used wasn't high enough) and during Pb elution (acid volume was too small). Differences between resins are for example different number of steps in resin preparation (Sr specific resin has the most steps and Pb specific has the least), the amount of solvents used (Dowex 1X8 uses the smallest amount), solvent used for Pb elution (Sr specific and Dowex 1X8 use HCl of different molarity, while Pb specific uses ammonium oxalate), etc. The advantage of Sr specific resin is that it allows the isolation of Sr and Pb simultaneously.

Since the separation efficiency for all studied resins is between 90 and 100 %, no Pb isotope fractionation is expected.

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Exposure to Cadmium in Slovenian population

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Human biomonitoring (HBM) is an effective tool for exposure assessment to harmful substances in human population studies. It also enables identification of susceptible population as well as subsequent effects on human health. The current study is performed on the population of primary school children from various potentially polluted areas of Slovenia. The purpose of our work is to present the current situation of exposure to cadmium in Slovenian children and adolescents and how the exposure differs between areas of residence, gender and age groups of children. The population of children and adolescents is considered the most susceptible to various environmental influences, as on average they are present and active in the outdoor environment relatively more than the adult population and consume larger amounts of food regarding their lower body mass and are consequently exposed to higher doses of pollutants as well. Our study is dealing with the exposure to cadmium in the general population of children and adolescents who are exposed to cadmium on a daily basis, mainly through water, soil and consequently food where concentrations are relatively low. Ultraclean sampling, sample treatment and analysis protocols were used followed by ICP-QQQ (triple-quadrupole inductively coupled plasma - mass spectrometry) as a detector, which is known for reaching very low levels of detection. Spatial and time trends will be presented, including recent sampling and analyses from previous campaigns. Moreover, the comparisons with national reference values for the adult Slovenian population will be done. Based on the questionnaires data (data on the frequency of certain food consumption which could be potential source of cadmium exposure, passive smoking and other life habits) and environmental data, the main sources of cadmium exposure in the investigated population will be presented. In addition, an association of Cd levels in studied population with the genetic predispositions of individuals will be done, since the internal dose of toxic metals in the body is influenced not only by the exposure to metals but also by mechanisms involved in their absorption, distribution, metabolism and elimination. With genotyping we will analyze some gene polymorphisms or SNPs (= Single Nucleotide Polymorphism), which were selected according to the literature and are believed to play a role in the mechanisms of cadmium uptake, metabolism and excretion. We will focus on metallothioneins (MT1A and MT2A), the transcription factor MTF1, the renal transporter CUBN, and the genes involved in the oxidative response to the presence of metals in general.

How can bacteria be forced to make useful biofilm?

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Attachment of bacterial cells to the surface and succession to the biofilm formation is often considered undesirable due to the colonization of surfaces by bacteria causing deleterious effects on surfaces or represent an increased health hazard. In contrast, biofilms are also desirable in the biotech process, where they are facilitating product separation and protecting cells from harsh environmental conditions. Many of the biotechnologically relevant strains lost their ability to the formation of biofilms and cannot be used in harsh conditions such as in the bioremediation approaches. Here we aimed to aid these bacteria to form biofilms using a physical approach. Since the attachment of cells is the most important stage of the formation of biofilm, we hypothesize that decreasing the distance between cell and surface will result in diminishing repulsive forces and will engage short distance acting as attractive forces resulting in the formation of attached cells. This will further promote the extension of cells in a parallel direction and the development of stabile biofilms.

For decreasing the energetic barrier, the transitional attachment of cells to the surface by the charge modification of cells by Layer-by-Layer (LbL) strategy was used. We used the same approach in strains that can or cannot form biofilm where we demonstrate that an artificial layer with the modified surface can be a premise for the biofilm formation even for cells that lack biofilm forming ability.

As a result, we achieved several findings indicating that (*i*) using LbL technology for surface modification allows using any bacterial cells to force them to form a biofilm, (*ii*) attached biomass is growing and dividing on the modified surfaces and, (*iii*) the surface modification does not introduce any toxicity for the bacterial populations. Since the biofilm formation is considered as a thread, we made a paradigm shift on assembling alive biofilm that prevents the attachment of pathogenic microbes, using a potentially probiotic strain of *Bacillus* sp. 25.2.M, which produces antimicrobial substances. Thus, the use of polyelectrolytes can be a versatile method allowing non biofilm-producing bacteria to form artificial biofilms with desirable composition.

Hydrophobization Study of Cellulose Nanofibrils Films with CF_4 plasma

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Cellulose is the most abundant polymer in the nature and is as such easily available, cheap and sustainable. It has a hydrophilic character that negatively affects water vapour barrier and limits its potential use as packaging [1]. However, it possesses reactive hydroxyl groups that can be modified. Various approaches to modification such as esterification, carbamation, silylation and click chemistry have been extensively researched [2]. However, little research focused on plasma treatment, which is quick and relatively cheap way to obtain hydrophobic surfaces.

With this in mind, cellulose nanofibrils (CNFs) films were treated with CF_4 plasma. Water contact angle was followed with respect to the treatment time (Figure 1). Samples were treated continuously or in five seconds intervals with intermediate five seconds cooling. It was found that already 30 s is adequate to reach hydrophobic CNF film. Furthermore, four samples that exhibited the most hydrophobic character (30 s, 45 s, 60 s treatment and 20 s in 5 s intervals with intermediate cooling), were selected and further analysed with SEM and XPS to observe structural change. The stability of modification after 3 days was tested as well and no change in the water contact angle was detected.

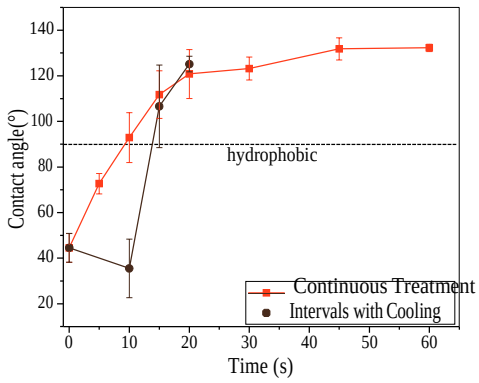

Figure 1: Water contact angle of the CNF films with respect to treatment time.

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Impact of *APOE* and *ALAD* gene polymorphisms on trace elements in pregnant women

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In everyday life, pregnant women are exposed to low levels of various nonessential trace elements (TEs) such as arsenic, cadmium, lead, mercury, etc. To mercury they are exposed particularly through amalgams and seafood intake while to lead mostly through diet. Furthermore, pregnancy can trigger the release of lead accumulated within the bones during previous life-long exposure. Levels of these TEs depend on many factors including the status of essential TEs and personal genetic background [1].

In the present study we investigated the relation between TEs and single nucleotide polymorphisms (SNPs) of apolipoprotein E (apoE; gene *APOE*) and δ-aminolevulinic acid dehydratase (ALAD; gene *ALAD*) in pregnant women in 2nd to 3rd trimester living in North Adriatic coastal region of Croatia (N=223) and Italy (N=900) (PHIME project participants). Mercury (Hg), lead (Pb), selenium (Se), and zinc (Zn) levels were determined in maternal whole blood (by ICP-MS) while Se and Zn were analysed in plasma as well (Se by ETAAS, Zn by FAAS). DNA was extracted and genotyped by qPCR using TaqMan probes for SNPs of *APOE* (rs429358, rs7412) and *ALAD* (rs1800435). ApoE is a lipid binding protein and it's three major isoforms (apoE2, apoE3, apoE4 — encoded by the alleles *ε2, ε3, ε4*) differently influence lipid and neuronal homeostasis as well as some processes related to their specific receptor binding, antioxidative and metal-binding properties [2]. ALAD is a Zn containing and Pb-binding enzyme involved in the haem biosynthetic pathway. Since *ALAD* rs1800435 polymorphism (alleles *ALAD1, ALAD2*) can influence the binding affinity of Pb towards ALAD, this may result in changes to the amount of bioavailable Pb in the body, as well as the severity of its effects [1].

TEs distribution between *APOE ε4* carriers and *APOE ε4* non-carriers and between *ALAD2* carriers and non-carriers was compared by applying Mann-Whitney U test (Table 1). Results were tested by multiple linear regression models (RStudio statistical software) ensuring all potential confounding variables such as age, body mass index, parity, fish intake frequency, smoking, etc. are incorporated. We confirmed positive impact of *ε4* allele on plasma Se in Croatian population (β =0.120) and negative effect on blood Hg levels in Italian population (β =-0.233). For *ALAD2* allele, the negative effect on blood Pb levels was observed and confirmed in Italian population (β =-0.086).

Table 1. TEs in whole blood and plasma samples for Croatian and Italian pregnant women.

CROATIA	***ApoE***			***ALAD rs1800435***		
	ε4+	*ε4-*	*p*	*ALAD 2+*	*ALAD 2-*	*p*
	GM, range, Me, (N)	**GM, range, Me, (N)**		**GM, range, Me, (N)**	**GM, range, Me, (N)**	
Whole blood						
Hg *ng/g*	2.61, 0.59 - 9.83, 2.85 (37)	2.02, 0.55 - 20.49, 1.93 (184)	**0.0165**	2.28, 0.61 - 9.71, 2.33 (31)	2.09, 0.55 - 20.49, 1.99 (172)	0.3413
Pb *ng/g*	12.84, 5.25 - 53.58, 12.78 (35)	12.02, 3.58 - 87.63, 11.55 (180)	0.4909	10.85, 4.34 - 87.63, 10.33 (28)	12.22, 3.58 - 55.46, 11.88 (169)	0.1081
Se *ng/g*	99.7, 67.9 - 142.0, 99.4 (35)	90.1, 42.4 - 182.4, 89.2 (180)	**0.0080**	90.0, 60.4 - 140.2, 90.4 (28)	92.6. 42.4 - 182.4, 92.1 (169)	0.4875
Zn *μg/g*	6.21, 4.58 - 10.27, 6.03 (35)	6.19, 2.90 - 11.04, 6.12 (180)	0.7283	5.88, 2.90 - 10.27, 5.88 (28)	6.30, 2.92 - 11.04, 6.24 (169)	**0.0765**
Plasma						
Se *ng/g*	61.7, 41.0 - 96.0, 62.0 (36)	53.7, 33.0 - 90.0, 54.0 (176)	**0.0006**	55.2, 43.0 - 72.0, 56.0 (31)	55.4, 33.0 - 96.0, 56.0 (171)	0.7931
Zn *μg/g*	0.75, 0.52 - 1.08, 0.74 (36)	0.76, 0.46 - 1.14, 0.73 (176)	0.8137	0.72, 0.46 - 0.94, 0.71 (31)	0.76, 0.52 - 1.14, 0.74 (171)	0.2645

ITALY	***ApoE***			***ALAD rs1800435***		
	ε4+	*ε4-*	*p*	*ALAD 2+*	*ALAD 2-*	*p*
	GM, range, Me, (N)	**GM, range, Me, (N)**		**GM, range, Me, (N)**	**GM, range, Me, (N)**	
Whole blood						
Hg *ng/g*	1.77, 0.23 - 20.31, 1.92 (126)	2.22, 0.05 - 39.6, 2.45 (728)	**0.0109**	2.01, 0.22 - 21.99, 2.32 (169)	2.20, 0.05 - 39.6, 2.42 (702)	0.2174
Pb *ng/g*	10.80, 3.60 - 60.46, 10.28 (121)	11.04, 3.09 - 48.44, 10.93 (687)	0.2315	10.20, 3.61 - 46.65, 10.41 (164)	11.21, 3.09 - 60.46, 10.87 (659)	**0.0483**
Se *ng/g*	117.3, 70.9 - 203.9, 116.1 (121)	120.4, 67.0 - 228.8, 119.1 (687)	0.1803	120.9, 78.5 - 201.8, 119.3 (164)	119.7, 67.0 - 228.8, 118.4 (659)	0.6641
Zn *μg/g*	5.22, 2.92 - 8.81, 5.17 (121)	5.23, 3.01 - 9.85, 5.22 (687)	0.8214	5.22, 3.65 - 9.85, 5.09 (164)	5.23, 2.64 - 9.70, 5.24 (659)	0.4246
Plasma						
Se *ng/g*	79.0, 50.0 - 105.0, 80.5 (120)	78.5, 45.0 - 118.0, 79.0 (704)	0.8292	78.1, 46.0 - 107.0, 79.0 (161)	78.7, 45.0 - 118.0, 80.0 (679)	0.5475
Zn *μg/g*	0.72, 0.56 - 0.97, 0.73 (119)	0.72, 0.52 - 1.00, 0.72 (702)	0.8660	0.73, 0.58 - 0.94, 0.73 (160)	0.72, 0.52 - 1.00, 0.72 (677)	0.4302

GM - geometric mean; Me - median; N - sample size; p - statistical significance of differences between polymorphisms ApoE and ALAD rs1800435 using Mann-Whitney u test; bolded $p < 0.1$; differences confirmed by models marked with red.

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Isotopes of Sr and Mg in a karst aquifer of the Ljubljanica River

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Authigenic carbonate has been recently proposed as the third major carbon sink after oceans and comparable to biological fixation. Many researchers have begun to undertake systematic research on rivers, especially the conversion transfer of CO_2 between the lithosphere, hydrosphere, and the atmosphere systems. However, the special connection between hydrological and biogeochemical processes regulating carbon dioxide fluxes in systems mentioned above is still unclear and has to be quantified.

Application of non-traditional stable isotopes of Sr and Mg, which co-precipitate with $CaCO_3$, allows us a new insight into material flows and mechanisms in the carbon cycle. The application of isotope ratios of elements, like Mg and Sr, in karst hydrology is based on fundamental mechanisms of element partitioning and their isotope fractionation during carbonate dissolution and precipitation in oxic and anoxic aquatic environments in karst conduits in aquifers, streams and river sediments.

The $^{87}Sr/^{86}Sr$ ratios of natural materials reflect the sources of Sr available during the formation, so the composition $^{87}Sr/^{86}Sr$ has been used for the identification of the origin and ground waters and as a tracer of water-rock interactions, bedrock weathering and mixing processes, while $\delta^{88}/^{86}Sr$ is used for identification of carbonate precipitation. Isotopic composition of Sr and Mg ($\delta^{26}Mg$, $\delta^{25}Mg$) was used in studies of carbonate weathering and C and metal cycling in aquifers and the formation of authigenic carbonate phases such as dripstone or fibrous microcrystal calcite, where considerable isotopic fractionation was observed.

The investigated Ljubljanica river aquifer, located in south and central Slovenia, can be characterised as a complex, hydrologically highly heterogeneous karst aquifer that has numerous springs and sinks and represents an interesting environment for studying hydrogeological processes. Because of the complex hydrogeological structure of the area, surface river flows are generally short; rivers and streams sink underground several times along the main flow paths.

The goal of this study was to obtain basic data on the isotopic composition of Sr ($^{87}Sr/^{86}Sr$, $\delta^{88}Sr$) and Mg ($\delta^{25}Mg$, $\delta^{26}Mg$) in potential sources of these two elements, i.e. in soil and bedrock, along with the isotopic fractionation of Sr and Mg during processes, leading to the formation of possible authigenic carbonates (leaching from the soil, dissolution of rocks, precipitation of carbonate). The $\delta^{25}Mg$, $\delta^{26}Mg$ and $\delta^{88}/^{86}Sr$ were determined by MC-ICP-MS, using DSM3 and NIST 987 as normalization standards for Mg and Sr, respectively.

Based on the isotopic composition of Mg and Sr in source materials, in karst springs and sinks and with the help of data on the isotopic fractionation of Sr and Mg during bedrock dissolution and carbonate precipitation, we assessed whether and to what extent the CO_2 fixation in the form of authigenic carbonate in the Ljubljanica aquifer occurs.

Monitoring of total mercury in air of the former mercury mine and in the vicinity of the cement production facility

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In the environment, the atmosphere plays a fundamental role in the mercury (Hg) cycle, facilitating the transport and deposition of this toxic contaminant. Three forms of Hg are considered in the atmospheric Hg processes, including gaseous elemental mercury (GEM) or Hg°, and two other operationally defined forms: gaseous oxidized mercury (GOM), which consists of some oxidized gaseous inorganic Hg^{2+} and Hg^{+} species and particulate bounded mercury (PBM), which consists of either oxidized Hg or elemental Hg associated with particles. The sum of all gaseous compounds and gaseous elemental Hg is referred to as total gaseous mercury (THg).

Unique chemical and physical properties of this interesting element determine its behaviour in the environment. Hg emission sources include natural, anthropogenic and reemitted processes unfolding in the biosphere. Natural sources of emission into the atmospheric air are an important element of its global fluxes and the largest element of the global Hg cycle. Geogenic activities such as volcanoes and geothermal areas, oceans, lakes, forest and contaminated sites contribute to Hg evasion in the atmosphere. Among global anthropogenic sources, most Hg are released from thermal power plants, metal (including gold), artisanal and small-scale mining, cement production, etc.

Quantifying atmospheric Hg concentrations is confronted with challenges, the most notable is the difficulty in measuring atmospheric Hg in low concentrations. However, there are several commercial devices available on the global market. Devices that are commonly used for air Hg monitoring are Tekran air Hg speciation system, PSA Sir Galahad, Lumex and many more. Even though there are limitations regarding these devices, they provide a good estimate and are used globally for atmospheric Hg studies. In this project, we quantify the atmospheric THg concentrations in Idrija, the former mercury mine and the cement production facility, Anhovo, located in Slovenia using three air Hg monitoring detectors, namely; the Tekran system, Sir Galahad and Lumex. Continuous Hg atmospheric concentrations measurements were performed using the Tekran system over one year (December 6, 2019–February 18, 2021), THg in lichen samples (*Hypogymnia Physodes*) were conducted for a period of 3, 6, 9 and 12 months respectively. Lichens were analysed after proper preparation by AAS detector Model Hg-201 Semi-automated Hg Analyzer. Total gaseous elemental Hg concentrations were measured using the Lumex detector with the results interpolated on a map with the application of ArcGIS software. Climatic factors which play an important role in atmospheric Hg concentrations data were characterized and used together with the results from the three monitoring techniques to determine the correlation between the measured THg concentrations and these interferences.

Natural recovery of the environment polluted by past mercury mining by studying the fractionation of mercury in river water

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Mercury (Hg) is a toxic metal with very specific and complex chemical and physical properties and that is superimposed on the strongly perturbed Hg cycle and the natural process of biomethylation that generates the bioaccumulating/biomagnifying monomethyl Hg (MMHg) form that we are all exposed to when we consume fish. In Slovenia, one of the biggest challenges is to manage one of the most mercury-contaminated sites in Europe, the legacy of the Idrija Mercury Mine, the second biggest mercury mine in the world, which was operational for five hundred years (1490-1995). During its operation, 127 000 tons (t) of Hg were extracted. Out of this, 37 000 t of Hg was lost to the environment, over 12 000 t of Hg entered the Idrija river system. An estimated 2 500 kg enters the river system annually and about 1 500 kg/yr transported to the Gulf of Trieste. Highly elevated levels of mercury compounds in all environmental compartments of the whole impact area of the Idrija Mercury Mine, due to centuries of mercury mining, have harmed human health as well as the entire ecosystem. Mercury behavior in the environment is very complex and we are far from the full understanding of the mechanisms and processes affecting Hg bioavailability, accumulation, and transfers in the geo and biosphere. The aquatic environment is particularly important for mercury transformation processes, which was proven in several measurement campaigns done so far in the study area.

One of the remediation options is the natural recovery of this contaminated site, the objectives of this study were to assess the concentration levels of mercury species in water after more than 25 years of closure of the Idrija mine, and to study seasonal and temporal variations of Hg species concentration levels by comparing the results with those measured more than 10 years ago to see whether the natural recovery of Idrija has been made and the changes of Hg fluxes over time. The objectives were achieved by performing monthly measurements (November 2020 to May 2021) of dissolved elemental Hg, reactive Hg, and total Hg (filtered and nonfiltered water samples) at the same stations as in previous campaigns to allow comparisons, to obtain ancillary data to assess water quality parameters DOC, SPM, T, pH, redox potential needed for the interpretation of data, and to implement statistical analysis to assess spatial and temporal changes.

Keywords: Idrija, river water, total mercury, reactive mercury, dissolved elemental mercury

Optimisation and validation of HS-SPME GC-MS method for the analysis of volatile organic compounds (VOCs) in dry-cured ham

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The numerous volatile organic compounds (VOCs) in dry-cured ham formed during complex biochemical and enzymatic processes are responsible for the final product's unique aroma and quality [1]. In this work, VOCs in PDO protected and non-specific dry-cured hams were identified using a rapid, sensitive and reliable method based on headspace solid-phase microextraction gas chromatography-mass spectrometry (HS-SPME GC-MS) [2]. A 50/30 μm divynilbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) SPME fibre was used to extract volatile compounds from the sample. The factors affecting the SPME process, such as equilibration (20-60 min), extraction (20-60 min), desorption time and temperature (40-70 °C) and salt addition, were optimised. The optimal SPME conditions were 60 min of equilibration followed by an extraction time of 40 min at 70 °C, and 4 min of desorption. In contrast, the results by sophisticated statistical Design-Expert® software have shown a slightly higher optimal extraction time (60 min). The method was validated by determining the linearity, limits of detection (LOD) and limits of quantitation (LOQ), working ranges, and method sensitivity [3]. The method was then used to analyse eight different samples from the Slovenian market. These included Slovenian Karst prosciutto (kraški pršut), dry-curred ham from the Krškopolje pig (only preserved Slovenian autochthonous pig breed), prosciutto made from pork of the Mangalica variety, Italian Prosciutto di Parma, and Spanish Iberico ham. Individual VOCs' were identified from their mass spectra by comparison to mass spectral libraries (NIST 14.0) and by comparing their retention indices (RI) and retention times (RT) with those of authentic standards. In total, 64 VOCs were successfully identified, among which aldehydes were the predominant group, followed by the fatty acids and alcohols. The developed method will help to determine quality among different hams from Slovenian and foreign markets.

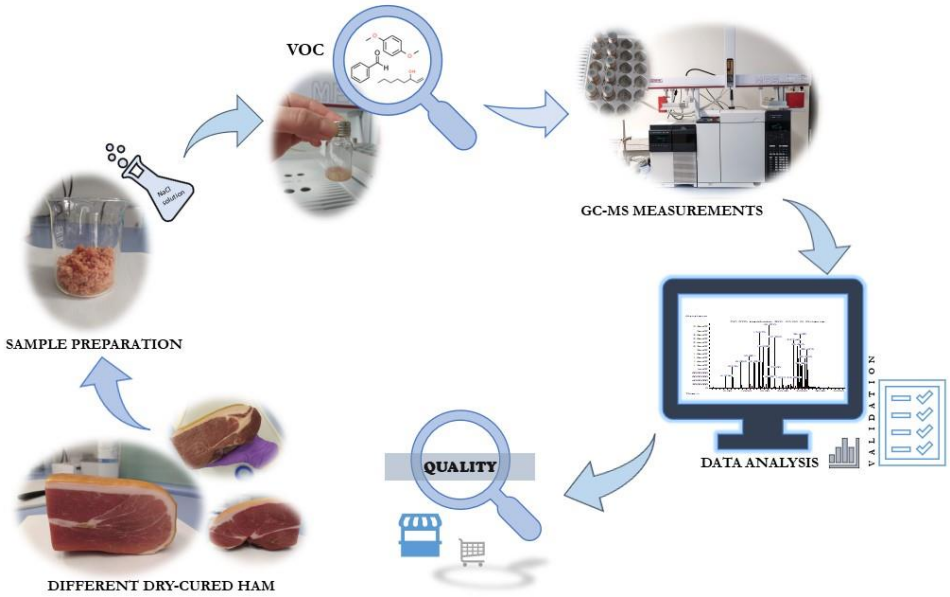

Figure 1. Graphical abstract

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Optimization of sample preparation procedures for Hg isotopic measurements

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Mercury is an element studied in many scientific fields, including geology, biology, oceanic and atmospheric chemistry, and other environmental sciences [1]. Its reactions and distribution can be traced by observing the stable isotopic ratios. Therefore, there are many different sample types, requiring different preparation procedures and with each one the fact that isotopes must not be perturbed should be taken into the account [2], [3].

Here presented are two digestion methods that gave some initially positive feedback. One used for lichens and the other for carbon and speciation traps used for collection of Hg from the stack. In the case of lichens, the material was digested in Teflon vials using concentrated HCl, HNO_3 and HF. To remove residual HF the contents of vials were evaporated for 5 h at 105 °C. NIST 3133 (solution), BCR 482 and IAEA 336 (both lichens) reference materials were used to check whether the digestion was complete. For ashes the pyrolysis was used. It was performed at 700 °C, the Hg vapour was then caught in an $KMnO_4$ trap. Here BCR-320R was used as the standard reference material.

To measure the Hg concentration Cold Vapour Atomic Absorption Spectrometry (Automatic mercury analyser HG-201) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) (Agilent 8800) were used. This ICP-MS was also used to perform a multi-elemental analysis. To measure isotopic ratios, Multi-Collector (MC-)ICP-MS was used (Nu Plasma II by Nu Instruments).

In the case of digestion, the final recovery was 84 – 89% (relative to the certified values of IAEA 336 and BCR 482) or 96% relative to NIST 3133. Multi-elemental analysis of IAEA showed the recovery for other elements was also in a similar range. When measuring the samples derived with pyrolysis the yield was 101 – 111%. The BCR 482 was also measured on MC-ICP-MS. There was no significant fractionation observed. It can be concluded that these methods are appropriate for use in sample preparation of lichens and ashes and could potentially be applied to other samples.

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Organic contaminants and where to find them

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Ever since the establishment of the term "Exposome", researchers have been aiming to assess the totality of exposure throughout the lifetime and its consequences. In Slovenia, Human Biomonitoring (HBM) has become a regular part of research. Among various monitored contaminants, selected were synthetic industrial chemicals and production by-products, such as persistent organic pollutants (POPs), phthalates, parabens, bisphenols, and triclosan. Exposure to these compounds mainly occurs via ingestion, inhalation, and dermal absorption.

As results from the 2011 DEMOCOPHES study suggest, plastic food packaging, PVC, and personal care products are important product sources for phthalate exposure of men, women, and children. However, factors like the level of education, living space, and time spent outside have significant impact on urinary concentrations of phthalate metabolites as well. As compared to other countries, the metabolite levels observed in Slovenia are well within the European range. However, phthalate exposure may pose a risk to the population when combined with other endocrine disruptive chemicals (EDCs), such as bisphenols, parabens, and triclosan. Thus, the hazard quotient (HQ) for the combined exposure to these contaminants has been obtained for the HBM I population (men and lactating women). The obtained values of 0.74 and 0.76 for women and men, respectively, do not exceed the HQ threshold of 1, indicating no risk at current exposures, but concerns regarding the 1) synergistic effects of other chemicals not included in the assessment and 2) individual susceptibility remain. Especially, the effects of single nucleotide polymorphisms on phthalate metabolism are currently being investigated for the HBM I population and preliminary results indeed indicate that carriers of CYP2C19 (rs12248560) variant allele express higher levels of certain phthalate metabolites in urine.

Additional reasons for concern are legacy contaminants that individuals are involuntarily exposed to mainly via diet. Exposure to POPs is ongoing due to their persistency and the ability to travel long distances. In Slovenia, local sources exist, so that these compounds were included in the HBM I study. The obtained concentrations indicate a very low POP burden. A preliminary hypothesis assumes that the Alps shield Slovenia from the long-range transport of contaminants via Westerly Winds, leading to lower concentrations of POPs on the lee side of the Alps as compared to the windward side.

At this preliminary state of results, we can conclude that exposure to chemicals in Slovenia is slightly below a magnitude where adverse health effects are possible. As such, we strive to deepening the current understanding of exposure by 1) the inclusion of more contaminants in the frame of ongoing HBM studies, 2) the assessment of individual susceptibility and 3) we aim at the development of robust analytical methods for the determination of contaminants in human matrices.

Unexpected exposure of children: Novel non-targeted screening workflow

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Environmental pollution has significant effects on human health. This is especially concerning for vulnerable populations, such as children which are in phase of rapid physiological changes. Unintended exposure to several chemicals has been linked to adversely affect children's reproductive system [1], neurological system [2] and even metal health [3].

To monitor exposure of children we usually look at predetermined compounds with known toxicity. However, by doing that we fail to see unexpected and potentially toxic new chemicals entering the environment in real-time. Non-targeted (NT) analysis aims at detecting every compound, facilitating real-time exposure monitoring for already known and newly emerging chemicals of concern.

Here we present a novel NT analytical method for global-scale exposure analysis and report preliminary results for Slovenian children.

As an exposure endpoint, urine of children, aged 6-9 years was collected. Samples were concentrated and purified using solid-phase extraction and separated using ultrahigh pressure liquid chromatography and detected using high-resolution mass spectrometry (Orbitrap Fusion). Data was processed using freely available MzMine 2.53, with parameters optimized for detection of low-abundance compounds. The resulting data matrix was mined using experimental and *in-silico* mass spectral libraries connected to feature-based molecular networking (FBMN). Compounds were identified using specialised identification software Sirius-CSI:Finger-ID, Metfrag and CFM. This analysis showed 77 contaminants, revealing high environmental burden of children. The children were exposed to pesticides, banned from use due to carcinogenetic potential, plasticizers with known endocrine disrupting properties and compounds deriving from personal care products with yet unreported concern for long-term chronic exposure.

The work presents an effective workflow for NT screening for organic contaminants in urine which was successfully applied to a study of children showing concerning exposure to, among others, restricted pesticides. These results raise concern for health of children and suggest inclusion of herein identified compounds into ongoing monitoring programmes.

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User experience and motivation of volunteers involved in environmental health studies based on low-cost air quality sensor technologies

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Technological developments in sensor technologies and wireless communications have contributed to the rise of low-cost environmental crowdsensing devices and applications [1]. Low-cost portable sensors are a current trend in citizen science (CS) projects that focus on air quality monitoring or exposure assessment democratizing air pollution monitoring [2]. Such datasets can provide information on exposure and increase community awareness towards air quality while providing scientists insights in environmental drivers on human health [3]. However, resource limitations in CS projects often require adopting suboptimal tools, which may come with hidden costs stemming from poor usability and underwhelming functionality, thus reducing volunteer's motivation [4]. Meeting the volunteers' expectations by designing or using existing tools with functional features which fulfil and nurture their motivations, will foster long-term participation and contribute to project sustainability [5]. Making sure that the tools used in CS are both of scientific value and provide meaningful information to the volunteers, requires user involvement in the design of the tools and services [6]. This contribution looks into studying user experience, their needs and motivations and gives examples how to conduct such studies.

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Using programming to increase the efficiency of microscopic measurements of biological objects

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Cell size has a great influence on the ecology of phytoplankton, because this characteristic affects the sinking rate, the susceptibility to grazing and the optimum for nutrient concertation through the surface area to volume ratio [1, 2]. Phytoplankton cell size and the associated biovolume are of critical importance in allometric studies[3, 4], furthermore body size offers potential advantages over standard taxonomic descriptors in community organization studies [5]. Despite its recognized importance, measuring cell dimensions in phytoplankton is not a straightforward process [5]. The main problems arise from the fact that this aquatic group is composed of unicellular organisms whose dimensions are on the order of a few to hundreds of micrometres and that currently the most widely used method for estimating the biovolume of phytoplankton cells is to assign each taxon a three-dimensional shape. The goal of this study is to provide evidence of how programming can reduce the time required for biological measurements while increasing the comparability of results and the accuracy of estimates by reducing errors in the procedure. The study presents the solution program written in Python 3.5 that provides the environment for the calculation of biovolumes and the computational solution to the thickness problem.

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What can U and Th isotopic composition tell us about environmental processes in karstic settings?

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Karst system is a challenging environment for studying environmental processes due to the heterogeneous geological and hydraulic framework. It is critically dependent upon hydrological conditions and climate change due to spatially and temporally variable water infiltration controlled by heterogeneous permeability [1]. In this complex setting, tufa could precipitate under special conditions, mostly in a turbulent stream at morphologic discontinuities and in lotic environments. Tufa's characteristics are influenced by the hydrochemical and climate evolution of river systems and can provide information on water-rock interactions, recharge, hydraulic connections, and terrestrial CO_2 cycle [2]. For better understanding the karst hydrodynamic system, we explored the spatial variability of U and Th isotopes in river water, surrounding carbonate-rich rocks and tufa and tried to identify and quantify authigenic carbonate formation in karst rivers.

River water, tufa, and surrounding bedrock and soil samples were collected at two different sampling locations, Krka River in Slovenia and Croatia, and were selected based on the spatial distribution of bedrock types and occurrence of tufa. Measurements of U and Th isotope ratios were carried out with multicollector inductively coupled plasma mass spectrometer (MC-ICP-MS) and for assessing U and Th concentrations, triple Quadrupole ICP-MS was used.

The results provided new evidence on the U and Th isotope disequilibrium in river water and its tufa appearance at two karstic locations. The differences in U isotope ratios and U concentrations within the watershed of both rivers are partly due to the different lithology and mixing of waters from different sources. Moreover, diffused groundwater discharge into the river can also contribute to the variability of the U isotopic composition in river water owing to water-rock interactions and the influence of the alpha recoil effect. Tufa samples display $^{234}U/^{238}U$ activity ratios similar to those of the river water, which were higher and relatively constant compared to the bedrock, springs and tributaries. This indicates that the majority of U present in tufa samples is co-precipitated with the carbonate from the river water and can demonstrate its authigenic origin. Additionally, Th and U concentrations and their isotope ratios in carbonate materials from both studies were shown to be reliable indicators of the storage of CO_2 as authigenic carbonate in tufa and a useful indicator for the determination of tufa with U bond to detrital material.

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Yeast lysate protein profile characterization by Orbitrap mass spectrometry: Effect of fermented *Spirulina* water or ethanol extract on yeast as a model organism

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Spirulina (*Arthrospira* spp.) is cyanobacteria with high bioactive compound and nutrient content with important therapeutic potential [1]. To enhance its bioactive and nutritional efficiency, lactic acid fermentation can be used, resulting in production of new metabolites from the original compounds [2]. Yeast cells are a good model organism for studying cellular processes and metabolic pathways [3], thus, in this study the lactic acid fermentation effect on Spirulina's bioactivity has been investigated, using water and ethanol extracts for yeast cell treatment.

Freeze-dried *Spirulina* samples were reconstituted and subjected to lactic acid fermentation using *Lactobacillus plantarum*. Water and ethanol extracts of fermented and non-fermented *Spirulina* were prepared for yeast cell culture treatment. Then yeast cell lysates were prepared to determine protein content using Bradford assay. Q-Exactive HF Orbitrap instrument was used for a comparative proteomic study of protein expression alterations between treated and non-treated yeast cells. To identify and calculate protein fold changes between conditions label-free liquid chromatography-tandem mass spectrometry coupled to data dependent acquisition was employed.

Preliminary results of the study showed significant differences in protein abundance between the yeast cells treated with water *Spirulina* extracts and ethanol *Spirulina* extracts as well as yeast cells treated with fermented and non-fermented *Spirulina* extracts. Significant separation was also noticed between treated and non-treated cells. Proteins with different abundance in tested conditions were further analysed using different bioinformatic tools to find cellular processes that are affected by Spirulina extracts. Among them protein biosynthesis, amino acid metabolism, carbohydrate metabolism and stress response dominated. Using proteomic approach, a better insight into Spirulina bioactivity was obtained.

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Informacijske in komunikacijske tehnologije (Information and Communication Technologies)

Condition monitoring of solid oxide fuel cells by a data-driven modelling approach

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A solid oxide fuel cell (SOFC) is an electrochemical device that with high efficiency converts the chemical energy of a fuel into electricity and heat. To get the required power on output, a suitable amount of fuel should be delivered on input. In normal operation, slightly more fuel than actually needed is delivered on the stack input. The percentage of the overall amount of fuel that is converted into electrical energy is referred to as fuel utilization (FU) and is normally around 0.75. Higher FU may cause oxidation of the anode and hence severe deterioration. The root-cause for increased FU is often in the fuel delivery system, therefore there is an obvious need for efficient online monitoring that can detect the problem in the early stage. The aim of our work is to create a system model in normal operating conditions, which is used for online monitoring in order to detect increased FU. The model is identified from input current and output voltage records obtained on the cell in a healthy state. Instead of identifying the entire system transfer function, the idea is to focus on the low-frequency part since the past investigations show that FU significantly affects the low-frequency part of the transfer function.

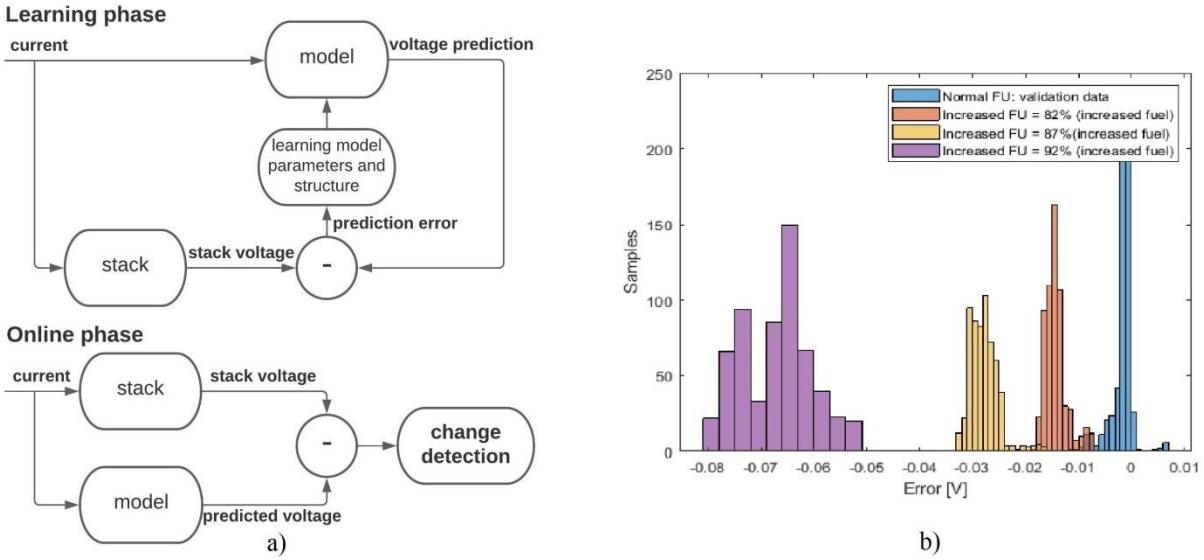

Figure 1. a) Off-line model learning and using the learned model in online monitoring; b) Results of the experiment: histograms of the model prediction error in normal (fault-free) operation and various grades of increased FU.

Subspace system identification method N4SID, realized in MATLAB, is used to derive a state-space model. The available information from the stack during the learning phase is used to create a model of the stack that will be able to make predictions for the output voltage. By comparing the stack voltage and voltage predicted by the model, it is possible to detect changes in the system in the online phase (see Figure 1a). The model error for normal FU is centred around zero while the increased FU model errors have shifted mean values and increased variances that are easily detectable, showing that the proposed setup clearly reacts to the increased FU (Figure 1b). However, the reason for increased prediction error might be also because of another degradation phenomenon and needs to be further studied.

ESTIMATING THE TIME A CLIENT STAYS IN THE JOB-SEARCH PROCESS

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The intense increase in popularity of the topics which consider modelling the labour market, analyzing ways to reduce the current state of unemployment, and creating a decision support tools are strongly due to the raise in the amount of digital data as well as the computational power. Creation of decision support systems and tools for organizations dealing with employment services directly supports the process of reducing the unemployment in the countries, which is a huge benefit for the overall economy. The aim of the paper is to analyze a machine learning (ML) based approach for modelling unemployed people that use the Public Employment Services (PES) to find a job. This work proposes an approach that emphasizes the deep understanding of the data and target variable, in order to create a specific model for tackling the problem. In particular, the goal is to develop a model for estimation of the time for a person to get out of the job-search process, after his initial entering to the PES. The dataset is complex and there is almost no pairwise correlation between most of the features in it, which makes it challenging for modelling. Statistical analysis and visualizations are performed in order to gain a better understanding and intuition about the problem and to form basis for further modelling. Having a prior estimation for the time a potential client uses the services of the PES, could be of great benefit for the selection process and resource management in the PES. Since the target variable for prediction is numerical type count data, the task is treated as regression problem. In this paper, a Univariate Poisson Deep Neural Network (UPDNN) model is proposed. The UPDNN model uses the minus log-likelihood of a Poisson distribution as a loss function, rectified linear unit (RELU) activation function in hidden layers for capturing nonlinear patterns and, in the output layer, the linear activation function for producing count estimate for the target variable. The proposed model is compared to classical machine learning models, such as linear regression, generalized Poisson regression models, Decision Tree models and Random Forest. As a result, several ML models are developed, one of which is a basic multiple linear regression that is used as a basic reference for performance comparison with other more specifically designed models.

Generation of a Priori Knowledge for Reinforcement Learning Using Neural Networks

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Reinforcement learning (RL) is widely used approach in robotics for refining the robotic skills. For some skills, it might take several tens or hundreds of attempts. These attempts are typically forgotten. In this paper, we show a method that uses neural network (NN) to store the knowledge about actions and action outcomes from all (successful and unsuccessful) attempts in order to provide a better initial approximate when the new action outcome needs to be learnt. Better initial approximation results in RL algorithm performing in fewer iterations or even becoming redundant when enough data about the task is gathered.

For accelerating RL learning process, we used combination of autoencoder (AE) network that was used for search space reduction and aforementioned NN used for accumulating the knowledge. Schematic structure of our approach is shown in Fig. 1 - left. Kinematic example trajectories were used to train autoencoder network that has a capability of extracting the main features of the trajectory (action) in its latent space. Small latent space is therefore used as a search space for RL algorithm. Information about all the executed pairs of latent space variables $\boldsymbol{\theta^{AE}}$ and action outcomes $\boldsymbol{q'}$ are stored in accumulator. After each successful iteration of learning (when $\boldsymbol{q' = q}$), the information from accumulator is used to retrain knowledge accumulating NN in several epochs and accumulator is emptied. Each time the new query ($\boldsymbol{q}$) needs to be learnt, knowledge accumulating NN is used to approximate the initial latent space values and only then RL is applied.

Our approach was tested on the example of robotic throwing action. Autoencoder network was trained on the kinematic database of throwing movements of Mitsubishi PA10 robot. In our case, movements were encoded as Dynamic Movement Primitives (DMPs), but any trajectory representation could be used. It was assumed that robot orientation is correct so only three joints of the robot that contribute to the shot in the saggital plane of the robot were used. Action outcome was to hit the target with coordinates $\boldsymbol{q} = [q_x, q_z]$. We performed experiments on learning to shoot at 200 random targets in simulation. After each target was successfully hit, NN was retrained. Error of the initial shot for each target is shown in Fig. 1 - right while the number of required iterations for learning of each target is shown in Fig. 1 - center. Both graphs show decreasing functions over the number targets, proving the benefits of our approach when storing the knowledge about the problems of the same type. In future, we plan to use this kind of NN to store the knowledge in simulation and to adapt them to the real world by performing only several RL examples.

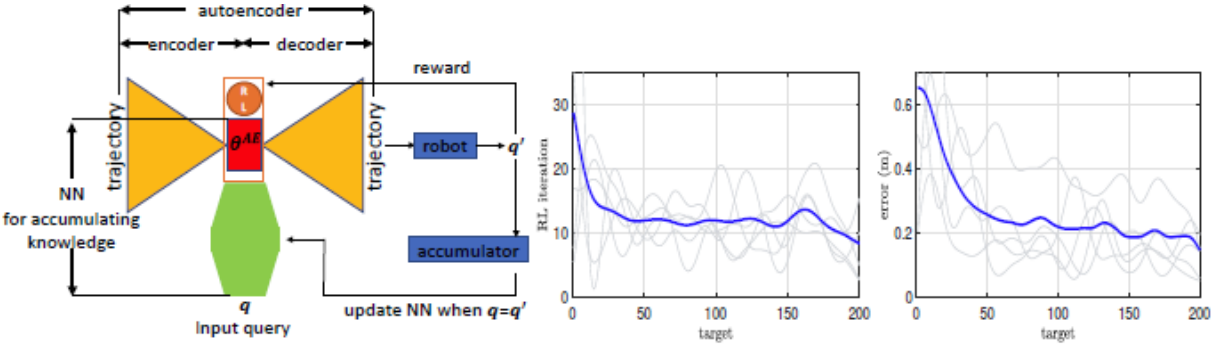

Figure 1: Schematic structure of the presented approach (left). Number of required RL iterations until the hit (center) and error in the initial approximate (right). All the results are averaged over 5 tests.

Testbed for a quasi-passive actuator for robotic exoskeleton

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There are millions of people who have limited mobility due to muscle weakness or injury. Years of evolution have led to very efficient bipedal locomotion in humans. However, when an additional heavy load is carried on the back, walking can be disrupted, eventually leading to muscle or tendon injury. Almost any change in the human musculoskeletal system increases metabolic costs. Current mechanical mobility aids do not fully restore mobility, which opens up a space for research in this area.

Exoskeleton devices have now advanced to the point where they can positively affect the mobility of healthy and disabled people[1], [2]. The development of such complex robotic devices brings together challenges from different research areas. The main challenges to be overcome are: lightweight and high power density actuation design, advanced control strategies, lightweight mechanical design, electronics and wearable sensors, new insights from human biomechanics.

Previous studies [3]–[4] have shown that by wearing a robotic exoskeleton and applying the right amount of energy at the right time in the gait cycle, it is possible to reduce the metabolic cost of walking. Existing actuators that are used are either passive, quasi-passive or active.

In this ongoing work, we are developing a modular experimental setup that will allow us to develop and test the quasi-passive pneumatic actuator with the mechanical force transmission mechanism. The main advantage of pneumatic actuators is the high weight-to-power ratio, but the main disadvantage is the need for an air reservoir, which limits them to the laboratory environment in exoskeleton applications. Simulation results have shown that we can avoid the need for an air reservoir by storing energy during one period of the gait cycle and returning it as needed during another period. The combination of the fast switching solenoid valves allows us to have the quasi-passive behaviour, but also the ability to change the parameters of the actuator. The developed prototype will later be used for the robotic lower limb exoskeleton, allowing us to develop advanced control strategies that collect data from wearable sensors and optimize the parameters of the actuator so that wearing the device results in reduced energy consumption while walking.

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Worst-Case Scenario Optimisation: Bilevel Evolutionary Approaches

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The bilevel optimisation problem is an optimisation problem, representing the upper-level and leader, which has as its constraints another optimisation problem, representing the lower-level and follower. Several challenges and complexities appear in order to reach the optimality of this problem. When no assumptions about the problem are made a solution is hard to find, leading the community to approach it both with classical and evolutionary methods.

Worst-case scenario optimisation – also known as min-max optimisation – is a special instance of the bilevel problem. It deals with the minimisation of the maximum output in all scenarios of a given problem. One can find these problems in optimisation under uncertainty, where the lower level plays the role of nature, that reacts to upper level's decisions in the most catastrophic way. Therefore, the upper level aims to find a solution that performs best even in the worst possible lower level's reaction. The most conservative but also the most robust solution is obtained by this approach.

There exist various Bilevel Evolutionary Algorithms (BLEAs) that have been tested and performed well on bilevel optimisation problems. These algorithms should also perform well in solving the worst-case scenario optimisation problem. Indeed, in our previous research [1], we tested 3 BLEAs on 13 min-max synthetic problems, where they reached the near-optimal solutions in most of the cases. The BLEAs tested are BLDE[2], BLEAQ [3] and BL-CMA-ES[4].

Extending this research, we apply them to a real-world engineering optimisation problem under uncertainty. The aforementioned problem is a simple truss design problem subjected to loads with uncertainty in magnitude and/or direction. The algorithms aim to find the optimal design under the worst-case scenario.

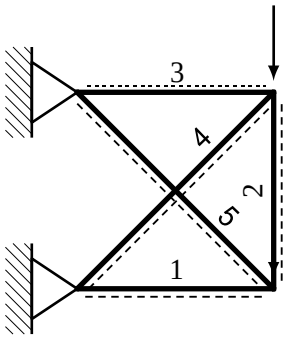

Figure 1: 5-bar truss design under loads.

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Nanoznanosti in nanotehnologije (Nanosciences and Nanotechnologies)

A DFT Study of Adsorption of Imidazole on Copper Surfaces Covered with Corrosion-Relevant Species

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Among a vast variety of different organic compounds, azoles—five-membered aromatic molecules containing one nitrogen atom and at least one other heteroatom (N, O, or S)—are known for their ability to reduce the corrosion rate of copper, i.e., they often act as corrosion inhibitors. It is generally accepted that molecules must adsorb on a metal surface to act as an inhibitor. However, in real environments metal surfaces are never clean. For this reason, we investigated how some adsorbed corrosion-relevant species affect the adsorption of azole corrosion inhibitors.

To this end, we performed a DFT computational study of imidazole—a building block of several efficient azole inhibitors—adsorbed on Cu(111), covered with either adsorbed hydrogen ($H_{(ads)}$), oxygen ($O_{(ads)}$), hydroxyl ($OH_{(ads)}$), or chloride ($Cl_{(ads)}$). Especially in aqueous media, the first three species are typically involved in cathodic corrosion reactions, while chloride is a well-known corrosion activator.

Our calculations reveal that bonding of imidazole on Cu(111) gradually increases with the increasing coverage of $O_{(ads)}$ by up to 0.5 eV in the case of the highest considered $O_{(ads)}$ coverage of ¼ monolayer. A similar trend was observed also in the case of $Cl_{(ads)}$, although the Cl-induced adsorption bonding enhancement of imidazole is smaller compared to that induced by $O_{(ads)}$. On the other hand, $OH_{(ads)}$ surprisingly reduces the stability of the adsorbed imidazole, whereas $H_{(ads)}$ does not have any significant effect.

According to our analysis, two factors contribute to the stabilization of adsorbed imidazole. The first one is due to formation of an H-bond between the imidazole and $O_{(ads)}$ or $Cl_{(ads)}$, whereas the second is due to enhanced direct N–Cu bond between the molecule and the surface. The latter effect can be associated with the ability of some adsorbates to alter the work-function of Cu surface, thus making the surface more susceptible to bonding with imidazole.

Calculations further reveal that in some cases co-adsorbed $O_{(ads)}$ and $OH_{(ads)}$ can promote the cleavage of the N–H bond in the azole molecule, resulting in an even more stable molecular adsorption mode. These findings raise an intriguing question regarding the nature and the extent to which some corrosion-relevant species affect the adsorption of inhibitor molecules.

Advanced Carbon-Nickel Sulphide Based Hybrid Electrodes for Lithium-Ion Batteries

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The exhaustion of available non-renewable energy resources is leading to an enormous demand for alternative energy storage options. Considerable efforts are being made to develop alternative energy storage resources and fulfil the energy needs beyond consumer requirements. Lithium-ion batteries are considered as one of the best performing energy storage resources with high specific energy and power density [1]. Even though, LIBs possess very high electrochemical features, there are lots of efforts have been employed to further improve the energy storage performances for the consumer needs. Among the various methods, one of the direct method to advance the performance of batteries is by using potential electrode materials. Transition metal sulphides are one of the potential materials for the next-generation battery electrodes due to their conversion-reaction induced charge storage mechanism [1], [2]. Though, poor conductivity and pulverization during cycling limit their applications as energy storage devices by limiting the cycle life, capacity and energy density. Consequently, a combination of metal sulphide phases with hierarchical carbon nanostructures is suggested to address these limitations. Moreover, the direct growth of electrode material on the current collector could give the possibility of producing binder-free electrodes. In this aspect, hybrid carbon-metal sulphide nanostructure directly grown on current collectors can be used as an advanced electrode material for energy storage applications. Herein, a fast, two-step approach is demonstrated for fabricating a hybrid electrode, consisting of trinickel disulphide (Ni_3S_2), metallic Ni nanoparticle and vertically aligned multi-walled carbon nanotubes (VCN) in the form Ni_3S_2/Ni@VCN. The VCN structure is prepared by plasma-assisted techniques, and the nickel sulphide is anchored by thermal annealing. As an anode for lithium-ion batteries, these Ni_3S_2/Ni@VCN electrodes exhibit outstanding lithium storage performance with a high reversible capacity, excellent long-term cycling stability, and good rate capability. The resulting electrode performance is one of the best lithium storage capabilities among the Ni_3S_2-based anode materials reported so far.

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Cold sintering: an efficient strategy to produce functional materials

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During the last several years, the Cold-Sintering Process (CSP) attracted increasing attention among scientists searching for novel routes of ceramic and composite sintering to form bulk components at drastically lower temperatures than with conventional high-temperature sintering. The CSP is a method still at its early stage of development, with researchers examining its applicability to a wide variety of materials and trying to understand the mechanisms that enable sintering without thermally-induced diffusion of atoms, and testing the possibilities of upscaling for industrial materials' production. This technique (schematically presented in Figure 1) utilizes high-pressure sintering (up to 600 MPa uniaxial pressure) of the ceramic powder, mixed with appropriate water solutions, at drastically lower temperatures, (from room temperature up to 300 °C). As a result, CSP enables to sinter dense materials (90 % of theoretical density and more). The main mechanisms that enable sintering at such conditions are mechanical compaction, followed by pressure- and solution-assisted dissolution of particles' surface, local diffusion of the species and precipitation of the compound, cementing the particles to form a ceramic.

There are several technological advantages of the CSP, starting with the possibility to get dense composites from phases that are difficult to obtain via conventional sintering (e.g., because of thermal instability of polymers, or because of reactivity between the phases that tend to form solid solutions, thus, losing the functional properties). Furthermore, the CSP is an energy-efficient method that brings significant advantages from ecology and economy point of view in comparison with different widespread techniques of ceramic sintering [1].

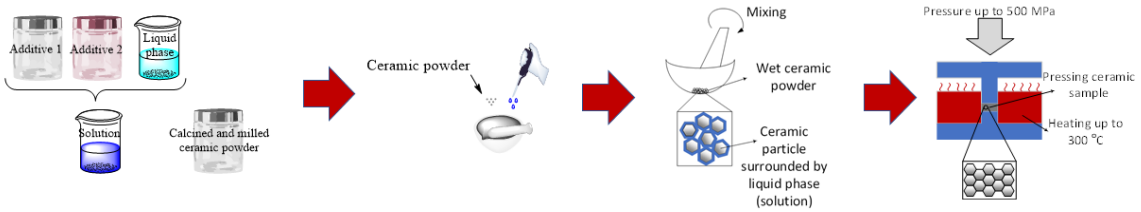

Figure 1 – Scheme of Cold Sintering Process

In this presentation we will show that the CSP technique can be used for sintering of several functional materials, also perovskites that are used as piezoelectric components. For that, appropriate initial powders and additives were chosen, followed by optimization of the sintering pressure, temperature and time. The effectiveness of sintering was determined by analyzing the structure and microstructure of the cold-sintered samples by X-ray diffraction, scanning electron microscopy, and measurements of materials densities. We will further show that cold-sintered perovskites exhibit ferroelectric properties via measuring of permittivity, losses, and polarization and strain as a function of an applied electric field. Our results confirm the opportunity to produce high-quality materials via the CSP.

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Corrosion stability of sintered and injection moulded ferrite-based magnets

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Permanent magnets (PM) are key elements in modern devices and enabling technologies as they allow storing, delivering and converting energy. Ferrite-based permanent magnets are in terms of volume one of the most used permanent magnetic materials in the world [1]. Good corrosion resistance is of great importance when it comes to the performance of PM. The goal of our study was to determine the corrosion stability of ferrite-based magnets produced in the course of the AMPHIBIAN project.

In our study, we tested sintered and injection moulded ferrite-based magnets using classical Engineering approach for corrosion testing. We tested the original material's magnetic properties, executed a corrosion attack and then remeasured the samples properties. Corrosion tests at increased temperature (80 °C) and humidity (100% humidity) for a prolonged time (100 h) were performed. To obtain our results, the properties of the material have been tested before and after corrosion by permeameter. The majority of samples displayed only a small difference in mass before and after corrosion tests, where the highest difference of 1.2% in mass before and after corrosion test has been observed for samples prepared from commercial strontium hexaferrite and consolidated by conventional sintering. We also measured a small difference in maximum energy product of some samples when comparing values before and after corrosion tests.

Since ferrites are high oxide ceramics a good corrosion resistance was anticipated in all of the tested samples. Based on the obtained results, we can say that ferrite magnets are suitable for use in conditions of elevated humidity and temperature.

Key words: Strontium hexaferrite, corrosion stability, magnetic properties, magnets

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Cyanine dyes for photothermal therapy: a comparison of carriers

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Cyanine fluorescent dyes are widely used as therapeutic agents. Indocyanine Green (ICG) is used for medical diagnostics and is investigated to be applied in cancer treatment as well. Unfortunately, it shows retinal toxicity [1] and there is wide concern about its systemic safety [2]. A similar dye, IR-820, has been shown to have lower cytotoxic values, higher solubility and higher stability [3], [4]. ICG is usually administered in isotonic solution for in vivo imaging purposes. Unfortunately, despite its excellent optical and imaging properties, ICG has low plasma stability, it is subjected to albumin binding, it is prone to thermal degradation, and its maximum of emission varies upon concentration [4]. Both dyes show also photothermal effect upon laser irradiation, that is desirable to apply in innovative cancer treatment. Encapsulation into liposomes might help reduce plasma degradation of ICG, extend circulation time and reduce toxicity [5]. We, then, compared photothermal effect of ICG and IR-820 in three different conditions: in phosphate buffer saline (PBS) solution (naked), encapsulated in lysolipid liposomes, and encapsulated in erythrocyte membrane-derived vesicles (EMV). The latter, taking advantage of their biomimetic nature, would help escape immune system recognition and clearance, while the encapsulation would avoid undesired side-effects and protect the dyes from photodegradation. Our results showed that both nanocarriers could protect from the degradation, quantitatively in the same way, of the dyes after the incubation 25ºC and 37ºC for 24 hours. Nanocarriers could not protect the dyes from photodegradation, that was comparable in terms of absorbance loss to the naked dyes. Photothermal effect has been observed for both dyes at two laser powers (0,5 W and 3 W), but ICG significantly has more heating ability than IR-820. Higher encapsulation efficiencies have been observed for both dyes in liposomes rather than EMVs, therefore higher photothermal effect. Further experiments will be needed to obtain definitive data about hemo- and cyto-toxicity of dyes, encapsulated or in PBS solution.

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Design of permanent magnets by solving the inverse magnetostatics problem

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Magnetic materials are used for permanent magnets, which are applicable, for example, in magnetic machines, sensors, or in magnetic recording devices. The additive-manufacturing technique makes the production of a single permanent magnet, specially designed for a particular application, possible. An essential step in design of a dedicated magnet is the reconstruction of the magnetization from the output magnetic field. This represents the inverse magnetostatics problem, which is ill conditioned due to the existence of multiple possible solutions. We present the adjoint approach, based on a reliable and stable solution of the forward problem by means of the finite-element method. The resulting magnetization state of a magnetic component can be tested by magnetic field measurements.

Keywards- Magnetostatics, ill-conditioned respective equations, inverse problem, finite-element method

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Hydrogen Evolution with $SrTiO_3/Bi_4Ti_3O_{12}$ Nanoheterostructural Platelets as Nobel-Metal Free Photocatalyst

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Increasing energy requirements, global warming and environmental pollution are some of the greatest problems of the 21st century. Production of storable and green H_2 fuel by using sunlight to drive chemical reactions over semiconductor photocatalysts is one of the promising solutions for these global challenges. At the current development stage, photocatalytic reactions still show low efficiencies mainly due to the high charge recombination rate, thermodynamically favourable backward reactions and narrow light response range of available photocatalysts [1]. Several design strategies such as loading of noble metal cocatalysts and/or formation of heterojunctions (heterostructures) have been proposed for the improvement of the photocatalytic performance [2]. Considering that noble metals such as Pt, Au, Rh and Ir are rare, expensive and harmful for the environment, our research is targeted toward the development of photocatalysts based on heterostructural systems. We have studied progressive topotactic replacement of $Bi_4Ti_3O_{12}$ precursor platelets with $SrTiO_3$ under hydrothermal conditions for the formation of novel $SrTiO_3/Bi_4Ti_3O_{12}$ nanoheterostructural platelets [3]. The partially replaced particles exhibit a tight contact between the $Bi_4Ti_3O_{12}$ template and overgrowing $SrTiO_3$ phase and highly ordered heteroepitaxial interface, beneficial for the charge carrier migration and separation. Measurements have shown that these heterostructural platelets exhibit 15-times higher photocatalytic H_2 evolution in water/methanol solution than commercial $SrTiO_3$ nanopowders even without the addition of noble metal cocatalyst [4]! Our results confirm that the production of heteroepitaxial particles using topotactic replacement under hydrothermal conditions is a promising approach for the preparation of novel heterojunction-based photocatalysts with higher efficiency. Through knowledge we can float toward a green new world!

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Importance of Deep Cryogenic Treatment in Present, Emerging and Future Industries

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In recent years, cryogenic treatment has been applied to improve properties of the steels in various emerging industries. Deep cryogenic treatment (DCT) is a treatment procedure, during which steel material is subjected to temperatures below -160 °C. DCT has been reported to influence the properties of ferrous and non-ferrous alloys, such as corrosion and wear resistance, hardness, fatigue, toughness, lifetime of tool etc. Simultaneously to the properties improvement, DCT allows also replacement of 2-3 cycles of tempering, which reduces the overall production costs. This study had taken under consideration a group of tool steels (under same DCT conditions), which are commonly used in emerging industries. Selected steel groups were systematically investigated for the contribution of DCT on their microstructural, mechanical, corrosion, wear and tribological properties. The study preformed a systematic evaluation and data collection of DCT influence on the properties of tool steels and unravelled certain mechanisms of DCT that have been unclear or unknown. The results evidently indicate DCT as an effective method for enhancing properties of materials used for industrial applications, such as medicine, automotive, aerospace, electronics, laser, 3D printing, magnetism, robotics etc.

Nanostructured ZnO for photocatalytic degradation of synthetic microfibers

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A large amount of the world's plastic by-products enters the ecosystem. This is creating the current pollutant crisis and is bringing about the term microplastic and nanoplastic. The words are used to describe a heterogeneous mixture of plastic particles smaller than five millimetres, differing in colour and shape (from different kinds of fragments, foams, pellets, granules, films to elongated fibres). Two types regarding the source are recognised. Secondary microplastics are a product of degradation of larger plastic debris exposed to various physical, chemical or biological stress. This fragmentation to smaller pieces is typical in landfill's soil and water environments. Primary microplastic consists of small particles of polymer-based additives originally manufactured in that size. They are used for drug delivery, cosmetics, clothing, industrial processes, and many other consumer products. In contrast, this type of plastic mostly enters the environment through wastewater system and spreads the oceans. In 2019, the World Health Organization (WHO) published a report where occurrence, potential health impacts, and removal of microplastics were critically examined [1]. The most common are; polyamide (PA), polypropylene (PP), polyester (PES) mostly polyethylene terephthalate (PET).

With this study, we represent an attempt to degrade microplastic fibers, released from washing machines, by photocatalysis as an environmentally friendly technique. PET, PA and PP microfibers were exposed to photocatalytic degradation. As photocatalysts, ZnO nanodots and nanorods were used. ZnO was prepared by hydrolysis and further hydrothermal treatment using zinc acetate, lithium hydroxide and absolute ethanol [2]. For characterization, XRD, SEM, TEM were used. For photocatalytic experiments handpicked microfibers were dispersed in a suspension of ZnO powder. Degradation was performed in an incubator, using simulated sun irradiation for 48 hours. Fibers were collected from the suspension, washed, dried and analyzed. Scanning electron microscope (SEM) analysis showed how surface of fibres changed after the photocatalytic degradation. We also include Raman spectroscopy, where we try to establish correlations between two methods. For future work, we expect to increase the rate of degradation process with proper doping of nanostructured ZnO.

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On a way to better understand the viral particles populations present in gene therapy drugs

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In recent years, many types of RNA and DNA viruses have been developed as recombinant viral vectors for the delivery of therapeutic genes to treat a variety of acquired and inherited diseases. Among them, adeno-associated virus (AAV) has shown great potential leading to the approval of viral vector-based gene therapeutics. In the production of recombinant AAVs (rAAVs), the harvest always contains a mixture of full, empty and partially filled viral particles. Downstream purification then focuses on the removal of impurities, but empty and partially filled viral particles are still present in the final drug product. In addition, a small fraction of full particles in the gene therapy product still contain heterogeneous fragments of unwanted DNA (e.g., host cell DNA, plasmid DNA), which may pose a safety concern, if not well defined or removed.

In our work, we compared the results of different analytical methods (transmission electron microscopy (TEM), cryogenic electron microscopy (CyroEM), transduction efficiency assay, digital droplet PCR (ddPCR), quantitative PCR (qPCR), and Enzyme-Linked ImmunoSorbent Assay (ELISA)) to gain a deeper understanding of viral populations in fractions recovered from the CsCl ultracentrifugation gradient.

Two different rAAVs (single-stranded AAV and self-complementary AAV) were produced and purified at International Centre for Genetic Engineering and Biotechnology (ICGEB) in Triste, Italy. Different viral particle populations and contaminants were directly observed using TEM by uranyl acetate negative staying and CryoEM, where viral particles were observed in native state, due to quick freezing in liquid ethane. The viral genome was determined by ddPCR, where 3 different set of primers targeted different parts of the viral genome. Commercially available kits (resDNASEQ Quantiative DNA Kit and HEK 293 HCP Elisa Kit) were used to assess the presence of host cell DNA and protein contaminations. Transduction efficiency assay was performed at ICGEB. We also examined the genetic content of the tested samples using the High-Throughput Sequencing (HTS) approach (Illumina).

The results showed many differences between the fractions and also between the two viral vectors. As expected, the optimal fraction containing the highest amount of full viral particles and the lowest amount of contaminating DNA molecules, was the full fraction. The intermediate fraction, which is normally discarded, also contained a high amount of full viral particles, which transduced cells with comparable efficiency as particles from the full fraction. The heavy fraction, which contained the lowest amount of vector genomes but a relatively high proportion of full viral particles, contained the highest amount of single-stranded host cell DNA. We have observed that both cryoEM and TEM are necessary for proper characterization of gene therapeutics and that HTS is a promising tool for impurities characterization.

Preparation and mechanical properties of low-adhesive high-strength composite material based on Polymer matrix reinforced with Al-based Quasicrystal powder

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Mechanical failures that may occur during space missions between two movable gears are attributed to tribological problems. Two movable joints that need to operate for long durations at very low torque and in extreme conditions can irreversibly degrade these components, resulting in loss of functionality. Through these challenges, we address the aim for the development of low-adhesive, high-strength composite materials that can prevent failure, which results from high-friction, fretting, and cold welding. First, we describe the preparation of low-adhesive polymer samples reinforced with Al-based quasicrystal (QC) powder. QCs can offer an excellent compromise between high hardness and low adhesion energy for non-stick applications [1]. The composite material was prepared by extrusion process to provide maximum homogeneity distribution of different volume fractions of QC particles in the polymer matrix. Mechanical tests were first implemented. The bending test showed that by adding QCs, we observed a linear increase of the maximum stress. Mainly, the maximum stress achieved for the pure polymer was 100 ± 0.5 MPa whereas for 5 vol.% and 20 vol.% of QCs addition into the polymer matrix, it was 102 ± 0.2 MPa and 112 ± 0.9 MPa respectively. The study of Vickers hardness of the composite materials showed that 5 vol.% of QCs added into the polymer matrix (15.8 ± 1.1 in Vickers) does not have a significant influence on the overall Vickers hardness (pure polymer 15.6 ± 0.1 in Vickers), but becomes significant when higher amounts of QCs are added in the system, for example 20 vol.% of QC powder (23.1 ± 2.9 in Vickers), Fig. 1.

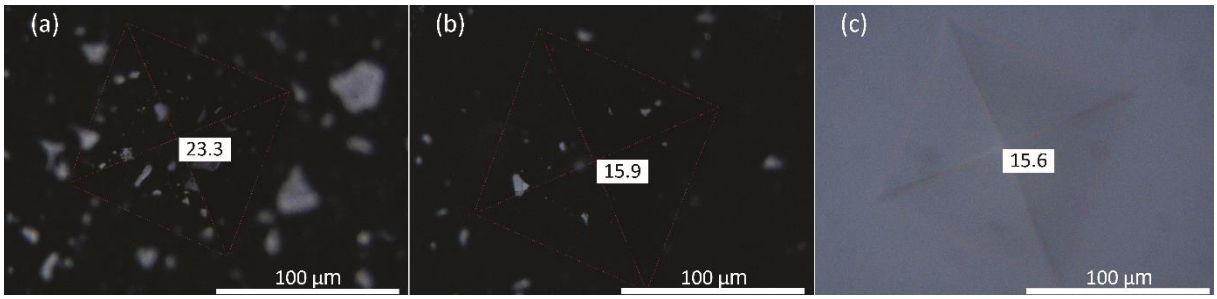

Fig. 1: Vickers pyramid of the material, which shows the hardness of the material. (a) polymer matrix + 20 vol.% of QCs, (b) polymer matrix + 5 vol.% of QCs and (c) pure polymer.

Acknowledgement

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Room temperature fabricated ceramic composites as future capacitors

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A ceramic capacitor is an important passive component integrated into various electronic devices, whose market is constantly increasing. In an attempt to meet the needs and expectations of global society and ecological standards, new technologies for the production of dielectric ceramics with improved functional properties gained a foothold recently. Room-temperature fabrication (RTF) is a promising alternative to time- and energy-consuming high-temperature sintering of electroceramics. [1],[2],[3] In the scope of our research bulk ceramic upside-down lithium molybdate-strontium titanate (LMO-ST) composites fabricated at room temperature are based on maintaining the high filler content and introducing a small amount of binder. A part of the binder is admixed to ceramic particles and additional part is added as a saturated aqueous solution, which crystallizes during pressing and drying. As the binder deposits at the surface of filler particles, the action of densification takes place. By virtue of that, a sufficient binding with 76 to 84% relative density was achieved. Thus far, the deeper insight in the method resulted from various processing aspects, along with corresponding microstructural analysis. The optimization of the particle size distribution, pressure, pressing time, ultrasound treatment, drying time, and processing conditions introduced improved functional properties of LMO-ST composites. In addition, we shed light on the investigation of the surface of ST, wetting, interfacial interactions and contact between binder and filler in order to further analyse and quantify the level of densification. Obtained experimental results of this study with relative permittivity in the range of 65–78 and dielectric loss tangent values from 0.002–0.05 in low frequency measurement range (1 MHz) can attract considerable attention for the utilization of LMO-ST composites in the industry of electroceramics. RTF entails almost infinite possibilities of a combination of different materials and the design of new composites with wide applicative value.

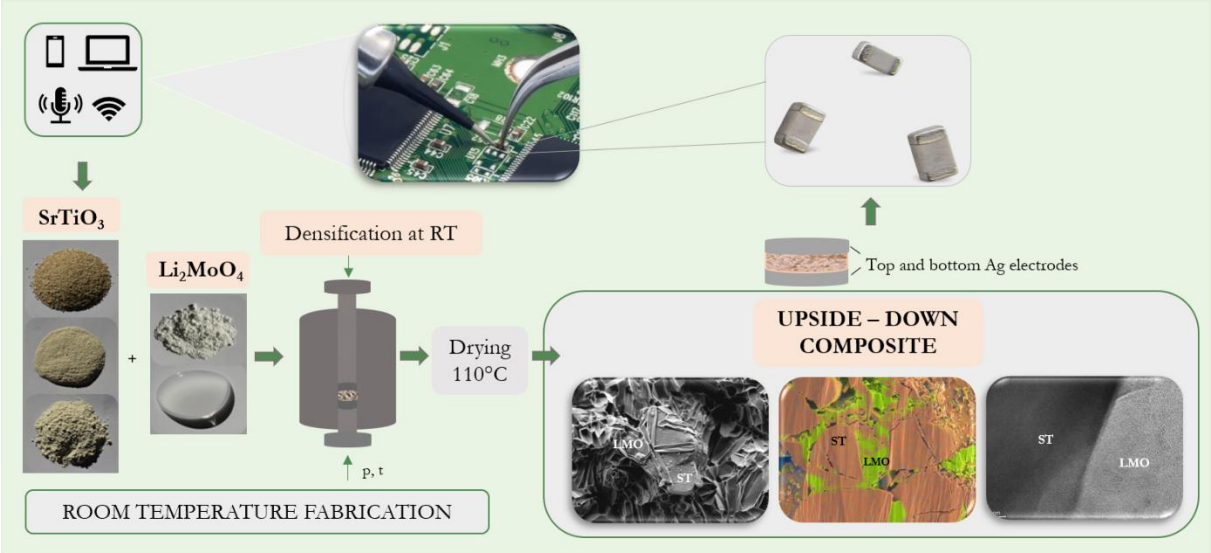

Figure 1. The experimental preparation protocol of upside- down LMO-ST composites

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Simple method to prepare piezoelectric nano-textured films for wound healing applications

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Use of soft piezoelectric materials to improve wound healing process (cell proliferation) is a novelty in the research field. The effect of electric stimulation, achieved through piezoelectrics, was shown to affect cell behavior [1] since it imitates the natural process of wound healing, where small electric fields are already present. Some researchers also state that electric stimulation acts against bacteria survival, which is a significant addition to piezoelectric films [2]. Poly-L-lactic acid (PLLA) polymer film is biocompatible and biodegradable and approved by the U.S. Food and Drug Administration (FDA) and the European Medicines Agency (EMA) for medical applications. It can also exhibit small piezoelectricity (10 pC/N) due to its asymmetry of polymer backbone and presence of C=O molecular dipoles, when prepared oriented and crystalline [3]. A simple method like "template wetting" can be used to prepare stretched and crystalline nanofibers or nanotubes [4], which is a requrement for a polymer to exhibit piezoelectricity. Anodised aluminum oxide plate (AAO) with well-determined nano-sized pores is used as a template, in which polymer is imprinted from the melt state. When using AAO template, oriented and slightly crystalline nanotubes are achieved on a polymer substrate, observed with SEM. After annealing above cold crystallization temperature, α crystals are confirmed using XRD method. With this approach, stretching of the polymer fiber occur due to capillary effect inside the tube in a template, therefore orientation in longitude direction is observed for the single nanotube using Raman spectroscopy. Since direct piezoelectric measurements of prepared nano-texture films are hard to achieve, piezoelectricity was indirectly confirmed through bacteria testing on *E. coli*. Comparing amorphous and crystalline nano-textured films, increased piezoelectricity was confirmed, when higher antibacterial effect was determined for annealed samples. Therefore, we expect that prepared nano-textured PLLA films are piezoelectric and can stimulate human cell growth while providing protection against bacteria.

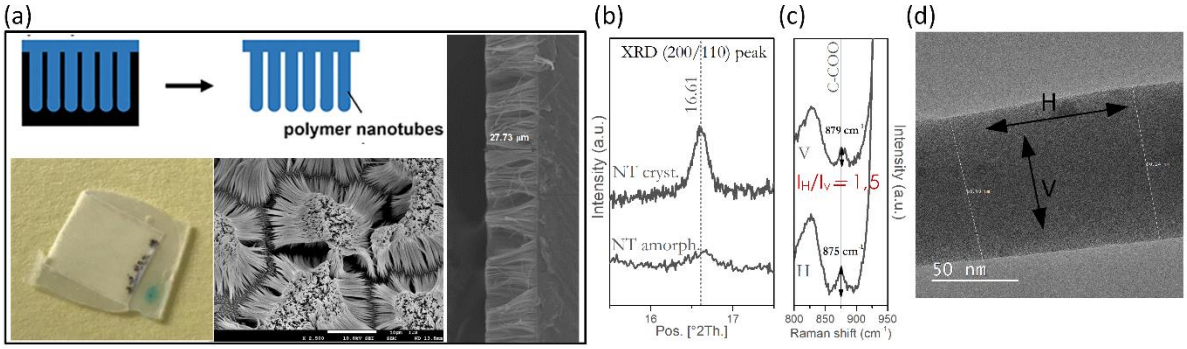

Figure 1. (a) Template wetting method with prepared sample (PLLA) observed from the top and cross-section; (b) XRD spectra of amorphous and crystalline nanotubes; (c) polarised Raman spectra of single nanotube; (d) TEM analysis of single nanotube.

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Suppression of the dissolution of $NaYF_4$-based upconverting nanoparticles at physiological conditions

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Upconverting nanoparticles (UCNPs) are due to their specific luminescence properties, promising alternative to conventional biolabels (i.e., organic dyes). Possible biomedical application includes bioimaging, diagnostics, and nanotherapy. The unique optical property is high-energy photon emission in the ultraviolet (UV), visible or near-infrared light (NIR), after the excitation with low-energy photons of NIR light (Anti-Stokes luminescence). NIR light penetrates deeper into tissues in comparison to organic dyes, excited with UV light (Stokes luminescence). In addition, multiple photon emissions are possible, with no background fluorescence or autofluorescence from tissues. However, the crucial step towards biomedical application is the biocompatibility of UCNPs. This includes nontoxicity together with chemical and colloidal stability of UCNPs under physiological conditions. All these requirements can be achieved with suitable surface modifications [1].

Our research focus are $NaYF_4$-based UCNPs co-doped with Yb^{3+}, Tm^{3+}. Their surface protection is essential due to their poor chemical stability and partial dissolution in aqueous media leading to possible toxicity [2]. Our aim was to develop protective coatings against the dissolution of the UCNPs. We selected amphiphilic polymer poly(maleic anhydride-alt-1octadecene) (PMAO), a copolymer of PMAO cross-linked with bis(hexamethylene)triamine (BHMT), and a phosphonate ligand ethylenediamine tetra(methylene-phosphonic acid) (EDTMP). The stability of coated UCNPs was assessed with dissolution experiments at physiological conditions (i.e., 37°C and 7.4 pH) in phosphate buffered saline (PBS), as one of the commonly used physiological buffers. Significant suppression of the dissolution was observed by the PMAO and PMAO-BHMT coatings. The long-term colloidal stability of the UCNPS coated with these two coatings was verified from the hydrodynamic sizes obtained with dynamic light scattering.

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Synthesis and characterization of $Li_{3x}La_{(2/3)-x}TiO_3$ ceramics for applications in all-solid-state batteries

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All-solid-state batteries represent a solution to the majority of issues related to batteries with liquid electrolyte used in conventional devices, regarding capacity, energy density, lifetime, size, and safety. Miniaturization of all-solid-state batteries is of great interest for researchers and industry as microbatteries are a promising technology for energy storage that can be used in portable devices, microelectronics and for medical purposes. Microbatteries can be fabricated with pulsed laser deposition (PLD) where high quality thin films with complex composition and selected morphological characteristics are produced. Materials with the best performance, i.e. highest Li-ion conductivity, are based on complex Li-oxides, such as $Li_{3x}La_{(2/3)-x}TiO_3$ (LLTO) [1]. LLTO is a double perovskite with the structure consisting of ordered La rich and Li rich layers along the $(001)_{LLTO}$ planes. A-site deficiency contributes to the high ionic conductivity that can reach values in the order of 10^{-3} S cm^{-1} at room temperature [2]. Ionic conductivity depends on the concentration of vacancies and Li content, the degree of A-site ordering and lattice parameters that can be adjusted by doping. It is known that Li ion can be transferred to the adjacent A-sites through the so-called bottleneck structure that consists of four oxygen ions and that the conductivity is higher along the Li rich layers [3], however, the exact mechanism of Li conductivity in LLTO is not fully understood. The aim of our research is to study microstructural aspects of LLTO in relationship to the La/Li ratio, processing conditions and doping in order to better understand the mechanism of Li-ion conduction. In our work we synthesized LLTO ceramic with different ratios of A-site cations using the solid-state sintering approach. We analyzed structural and microstructural characteristics of the samples with XRD, SEM and TEM and measured their functional properties related to the Li-ion conductivity.

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Synthesis of gold nanoparticles with atmospheric pressure plasma

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Sub-nm sized gold nanoparticles are the most frequent choice of material in potential applications starting from nanomedicine towards novel 2D nanoelectronics devices since it offers easy controllability of size and distribution, outstanding stability, and biocompatibility [1], [2]. A single step, atmospheric pressure plasma-assisted synthesis of nanocrystals of high purity gold directly from Hydrogen Chloroauric acid ($HAuCl_4$) has been demonstrated in this work. In this method, plasma allows direct modifications and direct reduction of the gas and liquid phase precursors inside the plasma. In conventional synthesis of gold nanostructure with well-defined geometries, the aqueous solutions of colloidal gold is used as precursors. In contrast with this, direct plasma deposition of $HAuCl_4$ solution yields nicely faceted metallic gold in nano-dimensions. The robust synthetic route with some significant advantages of this approach is described herein this paper. First, unlike other conservative methods of preparation of gold nanoparticles, plasma-enhanced vapour deposition is simple, highly reproducible and does not necessitate any external reducing agents. Since there are no external chemical agents, it does not require careful control of chemical conditions. Second, the prepared nanocrystals have a high level of purity without any defects without any later purification. Third, the surface of the gold nanocrystals on the substrate is accessible for linking other molecules. Therefore, we present a fabrication method of nanocrystals of gold on silicon wafer substrate, where they perform further growth and surface morphologies.

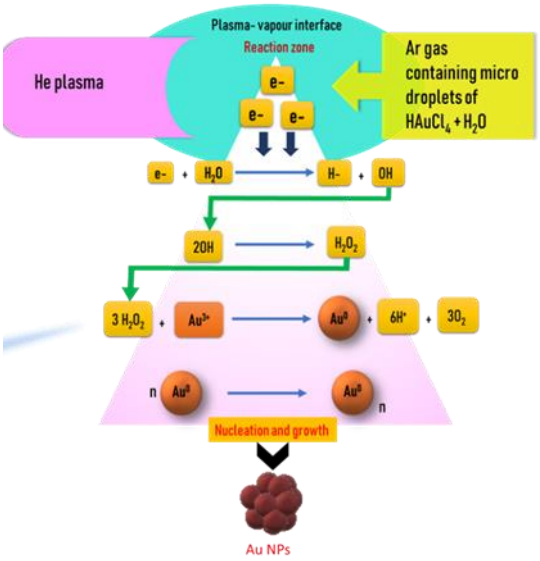

Figure 1. Mechanism of formation of gold nanoparticles inside plasma.

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The evaluation of effects on targeted high-throughput sequencing for the detection of bacteria and determination of microbiome in sputum samples

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The targeted approaches of high-throughput sequencing (HTS) have proven useful for detection of bacteria as well as the determination of microbiome based on sequencing of 16S rRNA regions. However, many factors can affect the results of HTS. To avoid potential mistakes during the research process that can lead to erroneous results, it is crucial to understand critical points in the workflow. In our study, we evaluated effects of commonly used DNA extraction methods on the detection of bacteria and determination of microbiome with targeted HTS in sputum samples.

Sequencing samples were prepared from sputum samples with normal lung microbiota collected at University Clinic of Respiratory and Allergic Diseases Golnik and spiked with *Acinetobacter baumannii*, *Klebsiella pneumoniae* and *Pseudomonas aeruginosa* in concentrations ranging from 10^3 to over 10^6 cells/mL as determined with turbidity measurements and corrected by digital PCR. DNA was extracted from the samples with three different methods: CTAB, GXT NA/Arrow, and QIAmp DNA mini kit in three technical repeats for each sample on two different days. Sequencing was performed using Ion Torrent Ion S5™ System and libraries were prepared with Ion AmpliSeq™ Library Kit 2.0 and Ion AmpliSeq™ Pan-Bacterial Research Panel. Raw reads after sequencing were analysed with Torrent Suite plugin PanBacterial Analysis.

The spiked bacteria in sputum samples were detected with 16S rRNA metagenomics and sequencing of specific amplicons for clinically-relevant species. The method using species specific amplicon sequencing was able to detect spiked bacteria in lower concentrations (down to 10^3 cp/mL) and in a higher percentage of samples compared to the 16S method. Differences between species were also observed. *P. aeruginosa* had consistently lower percentage of detection at the same concentration range than *A. baumannii* and *K. pneumoniae*. However, no significant difference between DNA extraction methods was observed for the detection of spiked bacteria. On the other hand, extraction methods did show significant impact on the microbiome determined with 16S rRNA metagenomics. Samples extracted with QIAmp DNA mini kit and CTAB consistently had the highest and lowest richness and diversity, respectively. Furthermore, many different taxa of bacteria showed to be present in different abundancies in samples extracted with different extraction methods. Beta-diversity analysis also showed significant differences between microbiomes of samples extracted with different methods.

The results of our study clearly show that DNA extraction method has an important impact on the microbiome determined with targeted HTS but did not have significant impact on the detection of spiked bacteria in sputum. On the other hand, the obtained results were repeatable which shows that targeted HTS gives reliable results and is a suitable method for the detection of bacteria and determination of microbiome in complex samples such as sputum.

The mechanism of glass-foaming with water glass

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Foamed glass is thermally-insulating material produced mainly for the needs of the construction sector. The possibility of using waste glass in its production is in line with new sustainability-oriented policies [1], making foamed glass a research-attractive material. Hydrous sodium silicate (i.e. water glass) is a common additive used in scientific investigations and commercial production of waste-based foamed glass. However, the mechanism behind the process aided by the water glass remains scarcely researched and was the main point of interest in this research.

Waste cathode-ray-tube (CRT) panel glass and water glass were mixed and analysed with heating stage microscopy. Gases that evolve during the heating were detected with thermogravimetry coupled with mass spectroscopy (TG/MS). Determination of the gases that remain trapped inside the pores was done with gas chromatography (GC). FTIR and XRD were used to analyse the material composition.

TG/MS and heating stage microscopy indicate that the expansion begins at the same temperature as a mass loss accompanied by the signal of CO_2. GC revealed that the pore atmosphere contains mainly CO_2. FTIR and XRD analyses show that a significant amount of carbonate species is formed during the mixture preparation. The foaming mixture was stored in the air or CO_2 before the heat treatment to further prove its sensitivity to the surrounding atmosphere.

The results of this investigation are surprising, almost contradictory to all the other literature regarding the mechanism of foaming with water glass. The obtained results suggest that the foams prepared via direct foaming method with the addition of water glass expand due to the formation of CO_2 and not H_2O.

Revealing the reactions of the foaming mechanism and the susceptibility to the atmosphere will be helpful in the optimization of any foaming process based on the use of water glass, with the potential to obtain a sustainable product with better performance.

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Thermoplastic 3D Printing of Ceramics

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Advanced engineering ceramics have good properties such as high hardness, chemical resistance and high mechanical strength, which make it possible for them to be used in many different areas namely medicine, chemistry and aerospace applications [1], [2]. But, shaping ceramics is a difficult task due to inherent inability of ceramics to plastically deform as well as the need for drying, debinding and sintering which is a process that allows densification at high temperatures. Until recently, ceramics have been processed by conventional methods such as pressing, casting and injection moulding, yet with limited geometrical complexity.
Introduction of additive manufacturing (AM) allowed processing ceramics into complex geometries with high precision. One of the many AM processes is thermoplastic 3D printing (T3DP), which is an AM technique that utilizes thermoplastic feedstocks allowing melting of the material with increased temperatures and solidification with decreased temperatures. This material property (thermoplasticity) allows efficient homogenization and dispersion of ceramic particles in the feedstock with high solid loading. In T3DP, a thermoplastic suspension loaded with ceramic powder (40-60 vol.%) is deposited in the form of droplets with the help of a piezoelectric microdispensing system. These droplets can be fused together by changing process parameters in order to result in formation of lines. The current literature on T3DP is limited since this is a relatively new process. T3DP process has large potential and is open for further improvement.
Aim of the presented work was to investigate the processing of ceramic suspensions by T3DP. Paraffin wax based ceramic suspensions were prepared by mixing and homogenization by 3 roll milling. The suspensions were processed by T3DP on a modified fused filament fabrication machine (HAGE 3D GmbH) equipped with a microdispensing unit (Vermes Microdispensing GmbH) to produce ceramic parts. Parts were investigated in terms of their density, porosity, mechanical properties and microstructure. As-prepared parts were thermally debinded and sintered. Density of parts was measured by Archimedes' method. Sintered bars were fractured by 4-point bending test and the results were analyzed by Weibull statistics. Microstructural analysis was made by SEM imaging.

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Tuning the magnetic and charge ground states of the Shastry-Sutherland compound $SrCu_2(BO_3)_2$ by chemical doping

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Low-dimensional quantum spin systems are materials which exhibit strong magnetic correlations in one or two spatial dimensions. In comparison to three-dimensional magnetism, the reduced dimensionality of magnetic correlations gives rise to a number of quantum phenomena and the possibility of obtaining exotic ground states of matter. A riveting example of low-dimensional magnetism is the strontium copper borate, $SrCu_2(BO_3)_2$. This compound is a frustrated quasi-two-dimensional spin system where $S = ½$ copper ions form a planar network of spin dimers – Figure 1a. It is the only known realization of the Shastry-Sutherland model and exhibits a sequence of magnetization plateaux at high magnetic fields [1]. $SrCu_2(BO_3)_2$ adopts a tetragonal structure with the $I\bar{4}2m$ space group where magnetic $Cu_2(BO_3)_2^{2+}$ layers are separated by non-magnetic Sr^{2+} layers – Figure 1b [2]. This study reports on the chemical doping of $SrCu_2(BO_3)_2$ with the aim of tuning its ground states properties. A-site doping with aliovalent ions is aimed, which could result in a free propagation of the singlets, leading to a *d*-wave superconductors. B-site doping, i.e. the substitution of Cu^{2+} with non-magnetic ions, is also envisioned. It could lead to breaking the spin dimers and to a possible realization of a quantum liquid of spin singlets. Polycrystalline samples are prepared by the classical solid-state method while single-crystal growth is performed by hydrothermal and flux growth. The characterization techniques used to investigate the newly synthesized samples are X-ray diffraction, magnetic susceptibility (SQUID) and neutron diffraction.

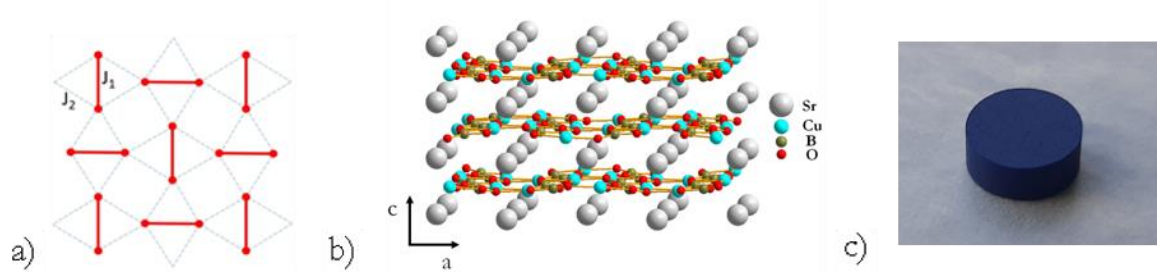

Figure 1. (a) The Cu^{2+} spin dimers within the 2D Shastry-Sutherland lattice; J_1 and J_2 are the intradimer and interdimer exchange interactions, respectively.
(b) A crystal structure of $SrCu_2(BO_3)_2$ is composed of $Cu_2(BO_3)_2^{2-}$ layers separated by Sr^{2+} layers.
(c) A typical $SrCu_2(BO_3)_2$ polycrystalline sample after sintering in O_2.

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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 first corrosion protection layer in the aircraft and automotive industry. Considering nowadays environmentally and budget-friendly CCs based on zirconium (ZrCC) and titanium (TiCC), parameters having the most influence on the resulting corrosion resistance, besides the substrate itself, are concentration, pH and conversion time. In particular, the main challenge remains to optimize new generation coatings to steel substrates [1].

Thus, in this work, low-carbon steel substrates will be subjected into a conversion bath containing hexafluorozirconic acid (H_2ZrF_6) and the aforementioned parameters will be optimized to give the highest values of polarization resistances obtained from a relatively rapid electrochemical measurement of Potentiodynamic Curves (PDC). Optimization will be performed using Response Surface Methodology (RSM), where a mathematical model of the system is created based on experiments performed according to statistically selected sets of variable combinations. The RSM plot shows both individual and mutual influences of the variables on the resulting response, from which optimum conditions can be easily predicted and tested [2].

After finding optimal conditions, the most scientifically appealing combinations based on electrochemical measurements will be subjected to further surface characterizations, such as Secondary Electron Microscopy (SEM) and X-Ray Photoelectron Spectroscopy (XPS) to get a better insight into surface composition and morphology as well as the substantial conversion mechanism.

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Senzorske tehnologije (Sensor Technologies)

2 years, 2 countries, 468 plants: a survey of tomato and weed virosphere in Slovenia and Serbia to equip virus diagnostics with a knowledgebase

Mark Paul Selda Rivarez[1,2], Ana Vučurović[1,3], Olivera Maksimović Carvalho Ferreira[1,2], Katarina Bačnik[1,2], Zala Kogej[1,2], Anja Pecman[1,2], Živa Lengar[1], Gabrijel Seljak[1], Ivana Stanković[3], Ion Gutiérrez-Aguirre[1], Nataša Mehle[1], Maja Ravnikar[1,4] and Denis Kutnjak[1]

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Disease outbreaks caused by emerging viruses introduced to a new plant host or region are preventable through strict plant health measures including surveillance through molecular diagnostics. However, classical diagnostic methods are reliant on the pre-existing genetic information of known viruses. Thus, to complement these methods, more information should be generated through extensive surveys coupled with a high throughput sequencing (HTS) approach. To achieve this, we conducted a two-year survey (2019-2020) of asymptomatic and symptomatic tomatoes and a variety of weed species surrounding selected production areas in Slovenia and Serbia, where a total of 468 plants were collected. Sequencing of ribosomal RNA-depleted total RNA extracts from the pooled samples was performed using an Illumina™ platform. Nucleotide sequences from sample pools were individually analyzed to detect viruses and construct genomes using a customized pipeline in CLC Genomics Workbench (Qiagen, v. 20.0) and SPAdes (v. 3.11). Virus genomes were taxonomically classified based on percent identities to known taxa obtained by nucleotide or protein based BLAST similarity searches, and according to the demarcation criteria set by the International Committee on the Taxonomy of Viruses (ICTV). We reconstructed genomes of at least 112 virus species, classified to 24 known virus families, of which at least 50 were assigned as putatively novel species. In addition, there were at least 30 virus-like sequences identified, which could not be classified to known viral taxa. The most abundant species in our samples belong to viral families: *Amalgaviridae, Aspiviridae, Betaflexiviridae, Bromoviridae, Closteroviridae, Iflaviridae, Kitaviridae, Luteoviridae, Partitiviridae, Picornaviridae, Potyviridae, Rhabdoviridae, Secoviridae, Tombusviridae, Tospoviridae* and *Virgaviridae*, indicating a vast diversity of RNA viruses in the sampled regions. In the Primorska region of Slovenia, where 48% of the samples were gathered, the highest numbers of viruses per location were detected, at a range of 14-30 viruses and virus-like sequences per sampling site. Overall, our current knowledgebase consists of biological and agroecological data, photographs of symptoms and the virosphere we examined contains at least 168 distinct genomic sequences. Using this vast information, we are now currently expanding our diagnostic capabilities by designing primers needed for laboratory detection to confirm these results and further investigation. We are also planning to further characterize selected viruses in terms of its infectivity in tomato or other solanaceous plants. These collected data will enable us to better understand the tomato and weed virosphere in the region, which can be used as baseline information for predicting virus emergence and outbreaks and other epidemiological studies.

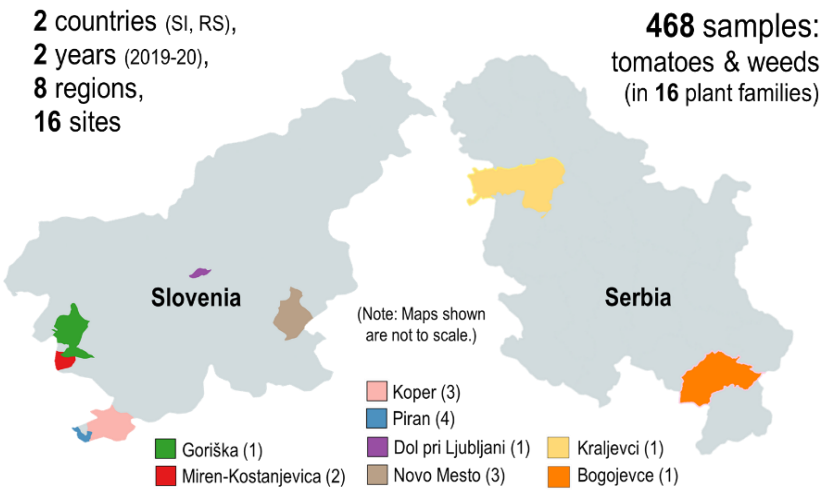
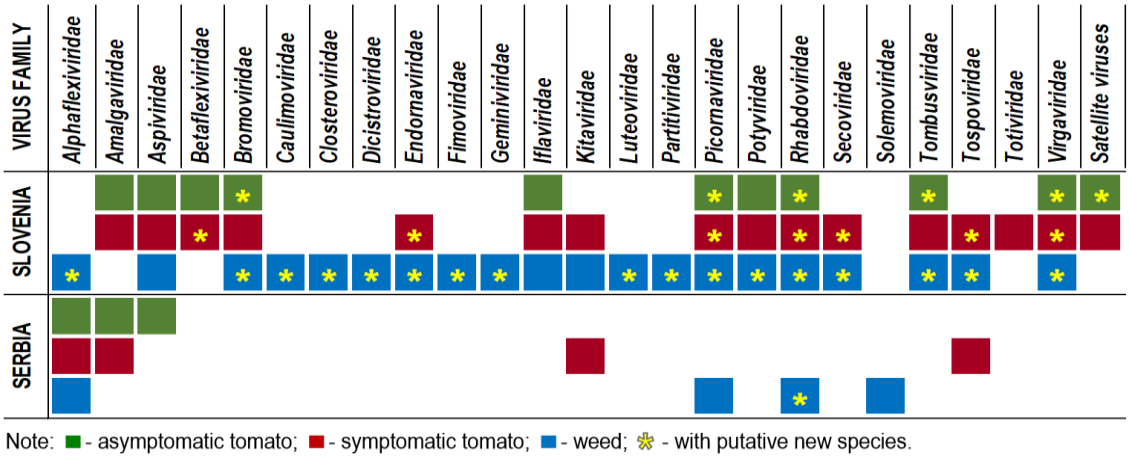


Figure 1. Regions where sampling was carried out. Number of sites visited are in ( ).

Table 1. Virus families identified.



Development and usage of detection test for '*Candidatus* Phytoplasma pruni'

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As the global population steadily increases and the threat of climate change rises, plant pathogens are becoming an important factor in ensuring food security. The development of rapid and accurate tests for detection of plant pathogens plays an important role in managing the spread of the diseases they cause. Phytoplasmas, wall less pathogenic bacteria that survive and multiply in the plant phloem and insect haemolymph, are one of most challenging plant pathogens for detection, because they cannot be cultivated. Taxonomically they are categorised into 33 groups based on their 16S ribosomal gene sequence. '*Candidatus* Phytoplasma pruni' ('*Ca.* P. pruni'), belongs to the 16SrIII group (subgroup A) and causes X-disease of stone fruit such as peach, apricot, nectarine, cherry and plum. The disease has serious impact on agricultural production causing complete loss of productivity and reduced life span of diseased trees. In western USA it has historically been a major limiting factors in peach production. When they reported 16SrIII-A phytoplasma presence in northern Italy and in addition, some '*Ca.* P. pruni'-related strains have been reported to cause damage to grapevines, we wanted to check its status in Slovenia. For this we firstly needed reliable, quick and sensitive test.

We designed primers and probes for TaqMan real-time PCR detection of '*Ca.* P. pruni' based on *secY* gene. With designed test we performed full validation: i) specificity testing *in silico* and experimentally, ii) sensitivity, with dilution curve of DNA extracts of 16SrIII-A phytoplasmas, iii) repeatability through analysis of three replicates of DNA samples with low, medium and high concentrations of the target and iv) reproducibility with testing on different days and with different machines. With this validated test we screened different field samples from different parts of Slovenia.

The designed test for '*Ca.* P. pruni' detection did not show non-specific hits to either phytoplasmas from other groups and other bacteria or to plant and insect hosts. With experimental specificity testing all of the 16SrIII-A isolates were detected. However, cross-reactivity was observed for isolates of other subgroups of 16SrIII. Therefore, for assigning subgroups we would need to do additional analysis. Test was shown to be able to detect low concentration of target phytoplasma and results were repeatable and reproducible. Afterwards we tested leaf veins of 434 symptomatic samples (grapevine, peach, apricot, apple, pear, and plum) collected between 2010 and 2019 in different locations in Slovenia and we did not detect 16SrIII-A phytoplasma [1].

Early and accurate detection of '*Ca.* P. pruni' and closely related strains is needed to prevent the spread of diseases they cause. The developed and validated test was shown to be a reliable and sensitive test that is useful for screening for '*Ca.* P. pruni' in large numbers of samples.

Reference:

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Investigation of domain walls in ferroelectric bismuth ferrite at the atomic scale

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Ferroelectrics are essential part of modern electronics as they are an active component in capacitors, ferroelectric random-access memories, sensors, transducers or actuators. Ferroelectric materials are divided in regions of different orientation of the polarization vector, regions called domains; the boundary between adjacent domains is called "domain wall" (DW) (Figure 1 a). DWs give an important, often dominating extrinsic contribution to the final functional properties [1]. Certainly, comprehending the chemistry and physics of DW is of high importance in the study of ferroelectrics. What has prevented so far a deep understanding of DW properties was a lack of high spatial resolution during investigation, as DWs are atomic-level-scaled topographic features. In fact, DWs have been interpreted, until the last two decades, in a very simplistic manner: as straight features without particular properties [2]. Excitingly, their complexity keeps revealing, especially as a result of the ongoing development of transmission electron microscopy techniques (TEM).

Motivated by the lack of DWs investigation in polycrystalline BFO and thus to the limited understanding of their local structure and chemistry, in comparison to their thin-film counterparts, in this contribution, we resolved the morphology and structure of DWs in $BiFeO_3$ (BFO) ceramic, by using atomic resolution scanning TEM (STEM) we show that DWs in BFO ceramic are not plain, straight features but they can form a step-like morphology (see an example in Figure 1 b) [3]. Further, a comparison between uncharged and charged DWs in terms of strain distribution, thickness and structure was performed and will be presented in detail [3].

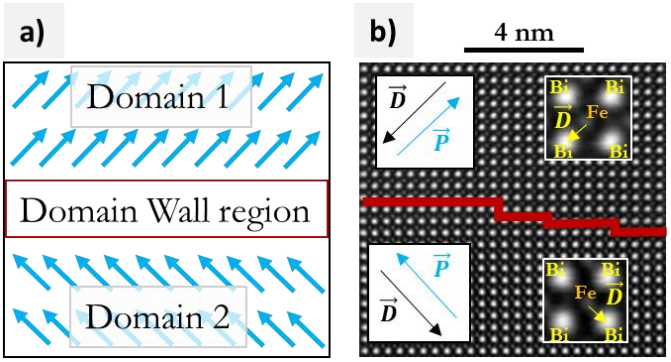

Figure 1. a) Organization of a ferroelectric in domains. Blue arrows mark the polarization vector. b) High Angle Annular Dark Field (HAADF) STEM image along $[100]_{pc}$ direction of step-like uncharged DW in polycrystalline $BiFeO_3$. The middle of the DW is marked with red line. The Fe-displacement vector in

respect with the Bi-sublattice with the corresponding direction of the polarization on each side of the DW is noted in the insets [3].

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Microstructural characterisation of ferroelectric $BaTiO_3$-based thin films

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Chemically modified $BaTiO_3$-based compositions have shown promise as ferroelectric lead-free materials, exhibiting comparable properties to the most commonly used $Pb(Zr, Ti)O_3$ [1]. Structural and microstructural details need to be obtained to understand and tailor the responses of these materials, making microstructural analysis a crucial step in the development of ferroelectric materials. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) are perfect tools for analysing the structure and microstructure of ferroelectrics in bulk as well as in thin film form. They cover a large size range from nanometer to micrometer scale and provide information on grain size, composition, crystallographic properties and domain structure. However, the insulating properties of ferroelectrics can complicate analysis, as the accumulation of electrons on the surface during imaging can lead to unwanted image distortion or artefacts. When using high-resolution field emission-SEM (FE-SEM) and TEM, the charging problem is usually solved by pre-coating the sample with a thin conductive metal layer or a carbon layer. Alternatively, in order to maintain resolution, samples can be analysed without pre-coating if a variable pressure SEM, also known as Environmental SEM (ESEM), is used, which allows imaging of non-conductive samples by neutralizing the surface charge with ionized molecules of the so-called imaging gas [2].

The aim of this study is the microstructural analysis of $BaTiO_3$-based thin films prepared by chemical solution deposition on platinized silicon substrates [3], [4]. FE-SEM, TEM as well as ESEM microscopes are used for the analysis. Preliminary results show that the ~300nm thin $0.5(Ba_{0.8}, Ca_{0.2})TiO_3$-$0.5Ba(Zr_{0.1}, Ti_{0.9})O_3$ (BCT-BZT) film consists of small grains with a size of tens of nanometers (Figure 1). In the presentation, the influence of the synthesis conditions (i.e. number of deposition layers, annealing temperature and time) on the microstructure of the $BaTiO_3$-based thin films is discussed and a comparison of the quality of the images obtained from carbon-coated and non-coated samples is made.

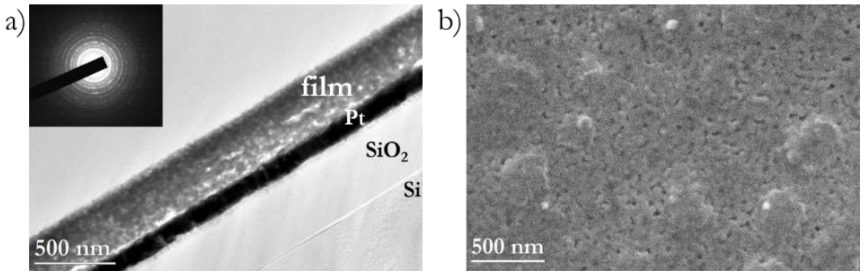

Figure 1. a) TEM cross-section image of BCT-BZT/Pt/SiO_2/Si thin film structure. Selected area electron diffraction pattern in inset confirms the polycrystallinity of the film, b) ESEM image of the surface of BCT-BZT thin film.

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Preparation of solid solution of barium titanate-based thin films by chemical solution deposition

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Barium titanate (BT) is a widely studied lead-free prototype ferroelectric material. The good electrical properties of BT-based solid-solution thin films such as $0.5Ba(Ti_{0.9}Zr_{0.1})O_3$-$0.5(Ba_{0.8}Ca_{0.2})TiO_3$ (BZT-BCT) could be an alternative to $Pb(Zr,Ti)O_3$ (PZT) for applications in actuators for micro-electromechanical systems (MEMS) or for energy harvesting. Among of methods of thin films preparation, Chemical Solution Deposition (CSD) is a simple method that enables the variation of composition or/and solvents and requires relatively low capital investments. Electrical properties of thin films prepared by CSD can be optimized by the control of microstructure properties and film-thickness. Conventionally, in CSD the main precursors used for coating solutions preparation of BT and BT-based solid solutions are alkaline earth carboxylates and transition metal-alkoxides. The former are dissolved in a carboxylic acid while the latter are dissolved in an ether-alcohol as it is shown in Figure 1a [1-2].
In this contribution, we propose a modification of the synthesis procedure of a series of BT-based coating solutions (BT, BZT, BCT and BZT-BCT) for CSD by introducing a diol solvent for the alkaline earth acetates according to ref. [3] as it is illustrated in Figure 1b. Importantly the shelf-life of the modified coating solutions has been extended from days to weeks. The mechanism of crystallization, microstructure characterization and the electrical properties of these films are investigated.

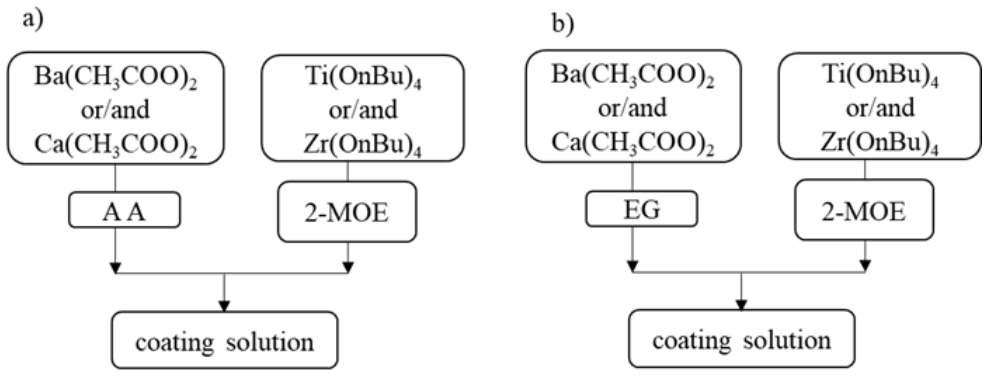

Figure 1. a) conventional method of BT-based coating solution preparation for CSD, b) proposed method of preparation of BT-based coating solution for CSD. AA: acetic acid, 2-MOE: 2-methoxyethanol, EG: ethylenglycol.

References:

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Relaxor-ferroelectric ceramic thick films integrated by aerosol deposition on metal and 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 substrates such as metals and polymers. In this context, relaxor-ferroelectric (1-x)$Pb(Mg_{1/3}Nb_{2/3})O_3$–$xPbTiO_3$ (PMN–100xPT) materials show excellent electro-mechanical properties, energy storage and energy conversion capabilities, suitable for electric generators, capacitors and electrocaloric cooling refrigerators.

In this work, dense 10 μm thick PMN–10PT films were deposited by the AD method on two types of substrates: low-cost stainless steel (Figure 1a) and flexible polymer substrates (Figure 1b). The powders were prepared via mechanochemical activation assisted synthesis, followed by additional thermal treatment and ball milling. Compressive stresses generated in the thick films during the AD process relax after thermal annealing at 400–500 °C. The annealed films attain a relaxor-like polarization vs. electric field hysteresis loops which makes them promising for energy storage applications. PMN–10PT films on stainless-steel exhibit a recoverable energy density of 9.8 $J \cdot cm^{-3}$ and energy storage efficiency of ~80% at 900 $kV \cdot cm^{-1}$. The films also exhibit high thermal stability and electrical field cycling stability up to 200 °C and $1.6 \cdot 10^7$ cycles, respectively. Furthermore, the relaxor-like behavior of PMN–10PT makes the films deposited on polymer substrate interesting for flexible electrocaloric devices. A detailed analysis of energy storage and electrocaloric properties of AD-processed PMN–10PT thick films will be presented in this contribution.

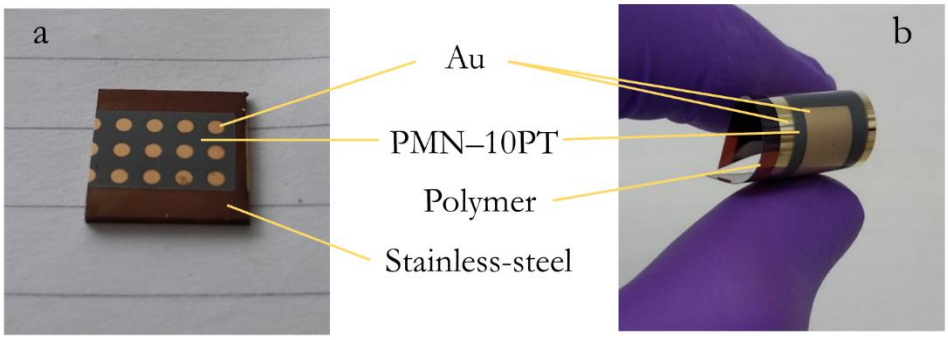

Figure 1. PMN–10PT thick films on (a) stainless-steel and (b) polymer substrates.

Wastewater surveillance for SARS CoV 2: deep dive into our society's health

Olivera Maksimović Carvalho Ferreira[1,2], Katarina Bačnik[1,2], Živa Lengar[1], Anže Županič[1], Mojca Milavec[1], Denis Kutnjak[1], Maja Ravnikar[1,3], Ion Gutierrez Aguirre[1]

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If the eyes are the mirror of the soul then a city's sewage is the reflection of its people's health. [1] Wastewater can provide us with a variety of information that directly speaks of the health and habits of the population. From use of illicit drugs [2], heavy metals [3] and antibiotic resistance genes [4] to detection of polio outbreaks [1], wastewater surveillance has already shown us its potential. The year of 2020 and the outbreak of SARS-CoV-2 virus have truly put the concept of sewage surveillance to the test. The world needed to rapidly adapt and accommodate large-scale population testing in the effort to contain the pandemic. Many countries, unfortunately, do not have the infrastructure to support this approach. As soon as it was confirmed that patients often shed virus through stool [5], wastewater surveillance came into the spotlight. Rapidly, various methods were published and several countries began pilot monitoring in key locations. For the particular case of Slovenia, we built on our previous experience in concentrating and detecting important plant and enteric viruses in wastewater, in order to establish a reliable monitoring strategy. New approaches were also evaluated, as higher throughput became more and more important. With solid workflows in place, we were able to monitor seven WWTP in Slovenia and a residence for the elder during the fall and winter in 2020-21, with coverage of approximately 600.000 people. Results obtained during the second wave of the epidemics highlight the positive correlation between results obtained from wastewater and clinical testing. Monitoring wastewater is therefore a valuable tool in terms of following the progression of the epidemics, impact of different measurements and the detection of hotspots in the early onset. Coupled with high-throughput sequencing approaches it is used for surveillance for mutations linked with novel variants of concern in the population, such as the B.1.1.7 variant (commonly known as the British variant) or novel viruses all together.

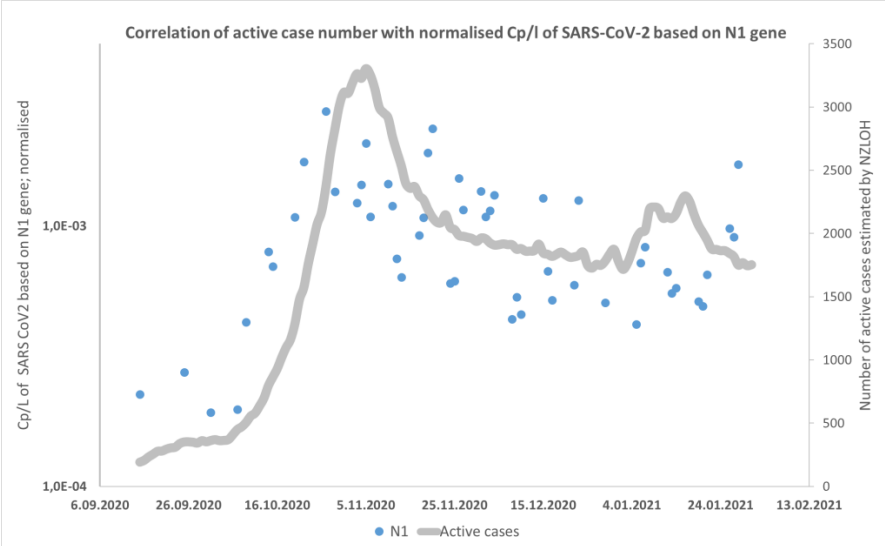

Figure 1. Correlation for WWTP Ljubljana

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Drugi programi (Other programs)

Advancing sample preparation through molecularly imprinted polymers

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Despite an immense progress in the development of analytical instrumentation, complex samples still require a preparation at a high degree of specificity, sensitivity and reproducibility. Sample preparation is both time consuming and can contribute greatly to the uncertainty of an analytical method. The complexity of sample preparation procedures depends on the sample matrix and analytical interferences, the concentration level of the analyte and subsequent instrumental analysis.

One of the more common sample preparation methods is solid phase extraction (SPE), which allows an efficient sample clean-up, preconcentration of the analyte and solvent modification in the sample. However, SPE depends on matching physicochemical properties of the analyte with the sorbent surface, resulting in general selectivity rather than specific extraction of the target analyte. But how can we increase the selectivity of extraction in sample preparation? The answer is hidden in the development of new materials with molecular recognition mechanism, i.e. the molecularly imprinted polymers (MIP), which are synthetic materials prepared in the presence of analyte template molecules that are subsequently washed away. Due to their exceptional selectivity and consequently improved sensitivity, robustness and precision, sample preparation with MISPE sorbents represents a significant advance over conventional SPE extraction.

Within this framework we synthesised a MIP for an active pharmaceutical substance bupivacaine. As a first step, different MIPs were synthesised using varying polymerisation ingredients at different temperatures. After removing the template their binding properties were assessed using high-performance liquid chromatography. The best performing MIP in terms of its superior affinity and capacity was then prepared at a higher amount. In the next step, the suitability of the MIP was tested for determination of bupivacaine in plasma samples of dogs involved in a pharmacokinetic study following tooth extraction. While at higher concentrations our material showed promising results, leaching of the template from the material makes the method ill-suited at lower levels. This can be solved by replacing the template with structurally similar analogue as a part of the MIP synthesis procedure, as will be discussed in the presentation.

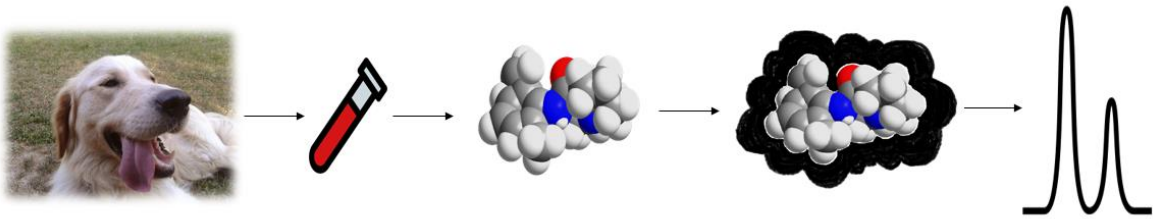

Figure 1. "Graphical abstract"

Antimicrobial components from avocado seeds for potential applications in medicine and food industry

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Natural sources rich in bioactive components such as enzymes, phenolic compounds and other phytochemicals are becoming increasingly popular. Some secondary metabolites represent great potential in the development of antimicrobial drugs as an alternative to conventional ones, as antimicrobial resistance is a major problem for public health. Due to their anticancer, anti-inflammatory, and antimicrobial properties, they have also become popular in recent years for use in the food industry to ensure food safety, in tissue engineering, and in biomedicine for wound healing and drug delivery [1]–[3].

Avocado is known for its beneficial health effects, but especially interesting is avocado seed, as currently represents an under-utilized resource and a waste issue. The seed can represent 20-30% of the total weight of the avocado, which means that, given the high consumption of the fruit, this also burdens the environment [4].

Due to the aforementioned facts, avocado seeds have been used to obtain bioactive components that exhibit antimicrobial properties. Bioactive compounds from avocado seeds were obtained by classical isolation and by using green technology - technology with supercritical fluids. A study of the antimicrobial efficacy of the obtained bioactive compounds from avocado seeds was performed. The antimicrobial efficacy was tested on various types of bacteria (Gram-negative and Gram-positive) and fungi, which are the main representatives of microorganisms that are transmitted by food, colonized during food-packaging, or pose a problem in antimicrobial resistance.

The results of the study showed that bioactive components from avocado seeds obtained by different isolation methods can inhibit the growth of 13 of the 15 different types of microorganisms tested.

The use of waste avocado biomass represents a great opportunity for development of the added value products and ecological opportunity, as well. Its use could thus help to protect nature and contribute to more sustainable production methods. Therefore, it makes sense to use it sustainably to make high value products that could be used in biomedicine or in the food industry.

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Development of an analytical method for the determination of bisphenols in activated sludge and their fate during conventional wastewater treatment

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Bisphenols (BPs) have been widely applied in the industry as monomers in epoxy resins, and polycarbonate production. They all share a common structure of two hydroxyphenyl functionalities and are known to have endocrine-disrupting effects. They have now been detected in surface water, sediment, sewage, and sludge, and several of them (BPA, BPF, BPS, etc.) should be considered as contaminants of emerging concern. For this reason, our research aim is to understand the fate of BPs during conventional wastewater treatment. According to their different known physico-chemical properties, their distribution between the aqueous phase and activated sludge should be investigated and their adsorption and biodegradation potential determined to evaluate their emissions to surface waters *via* an effluent release or an activated sludge disposal. An in-house method for the determination of BPs in the aqueous phase has been already developed. Currently, an analytical method for the determination of eighteen BPs in activated sludge has been developed and validated, based on solid-phase extraction (SPE) and gas chromatography-mass spectrometry. The method was optimised by comparing different SPE protocols for BPs, three of them based on hydrophilic-lipophilic balanced (HLB) copolymer sorbent and one of them based on molecularly imprinted polymers (MIPs) sorbent (Figure 1). The SPE procedures based on HLB Prime cartridges differed in the treatment of the extract before loading on the cartridges, as follows; (1) the extract was not refined, (2) the extract was prefiltered, and (3) the extract was precleaned using QuEChERS. The first protocol yielded the highest recoveries (≈ 91%), good repeatability, was the least time consuming and most cost effective. The analytical method will be applied to the full-scale wastewater treatment samples to evaluate the amounts of BPs adsorbed to activated sludge. The influent, and effluent samples will be analysed in an attempt to close the mass balance. Experimental results will be compared to those obtained by modelling.

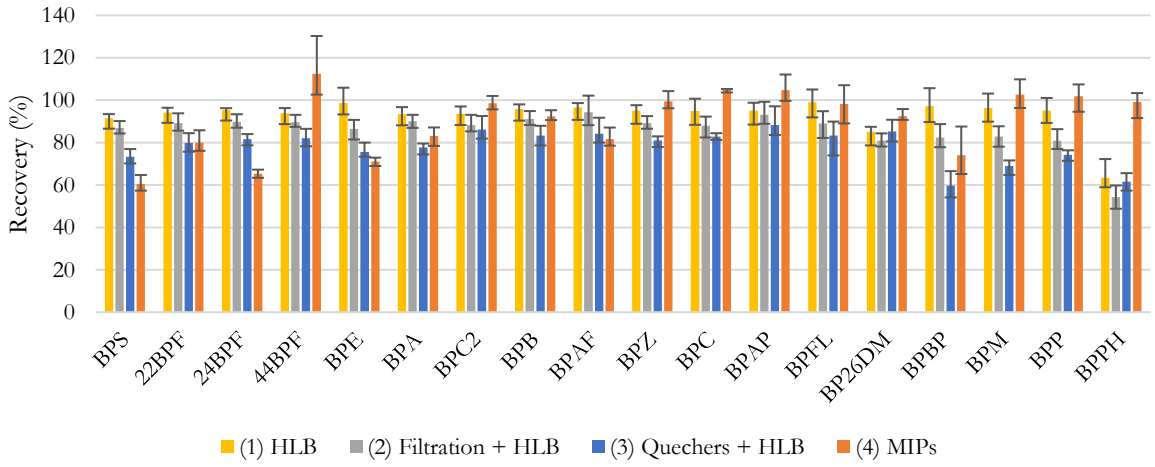

Figure 1. Recoveries of 18 bisphenols obtained by four different protocols for sample preparation.

Difference in adaptation to force field perturbation during hand reaching movement with random or alternating sequence of perturbation directions

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When subjects perform reaching movements and are subjected to perturbations, they gradually adapt their movements [1], [2]. If they are subjected to two different perturbations (e.g. in left or right direction) they cannot easily switch between them [1], [3]. However, some researchers suggest that switching between different perturbations is possible if subjects are given sufficient contextual cues about the change [4]. This study also suggests that it is easier for subjects to adapt to a random sequence of the force field directions than to an alternating sequence [4].

We hypothesise that random sequence of perturbation direction helps subjects to pay more attention to the task than during the alternating sequence of perturbation. In our study, subjects were making hand reaching movements with a perturbation in the left or right direction. The goal of the study was to compare how subjects perform the task during alternating and random sequences of perturbation directions.

During our experiment, subjects were sitting in front of a screen, holding the handle of a haptic robot, which was located under the screen as seen in Figure 1A. Their goal was to hit the target which was located 10 cm away from the starting position. Velocity dependent force field was used as a perturbation.

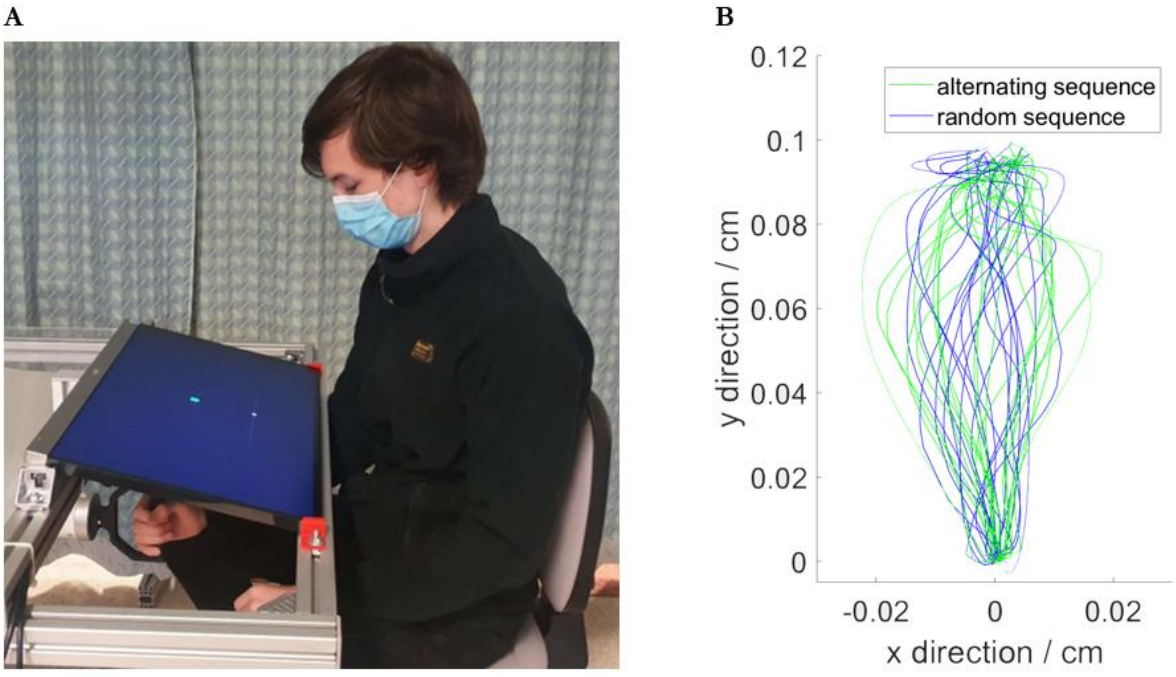

Figure 1. A) Experimental setup, B) trajectories during alternating sequence in green and during random sequence in blue.

Subjects first performed a block of trials with perturbation in one direction followed by a block of trials with perturbation in the other direction. At the end, there was a set of trials with a predetermined sequence

of perturbations in the two different directions that were meant to test if subjects can switch between the two different force fields. This final sequence consisted of a random and an alternating part.
Figure 1B shows exemplary results from one subject, comparing alternating and random sequence. We can see that on average, the trajectories during the alternating sequence deviate more from the straight path than the trajectories during the random sequence.

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Electric field driven reconfigurable nematic topological defect patterns

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Topological defects (TDs), in which the relevant order parameter field becomes ill-defined at a point, line, or surface [1], appear as a consequence of continuous symmetry-breaking phase transitions. As they generate complex order parameter patterns, TDs are relevant in diverse areas such as particle physics, condensed materials, and cosmology, with TD-dominated physical properties exhibiting universal behaviour independent of the systems' microscopic details. However, stabilization and manipulation of TDs is notoriously difficult. Moreover, their controllable and multistable manipulation among predetermined configurations is scarce, and in particular has been completely unexplored for ubiquitous "chargeless" defect lines. Here we demonstrate the systematic assembly and reassembly of a lattice of line defects in a thin nematic liquid crystal (LC) cell that is nanopatterned for orientational order [2]. We present robust experimental and theoretical frameworks in which an external electric field is used to switch between pre-determined and stable line defect configurations by coupling the field to the complex director profile surrounding the defects. Owing to their large response to external stimuli and large optical and electric anisotropies, liquid crystals provide an ideal test bed for many topological-based phenomena and encourage manipulation of TDs over a wide range of scientifically important systems, such as superfluid vortices in 3He and 4He, Bose-Einstein condensates, and Abrikosov vortices in superconductors. We anticipate that our proof-of-concept for "rewiring" topological line defects in liquid crystals also may lead to a variety of applications based on reconfigurable nanowires in soft matrices such as multistable optical displays, electronics, and charge carrier pathways for photovoltaics.

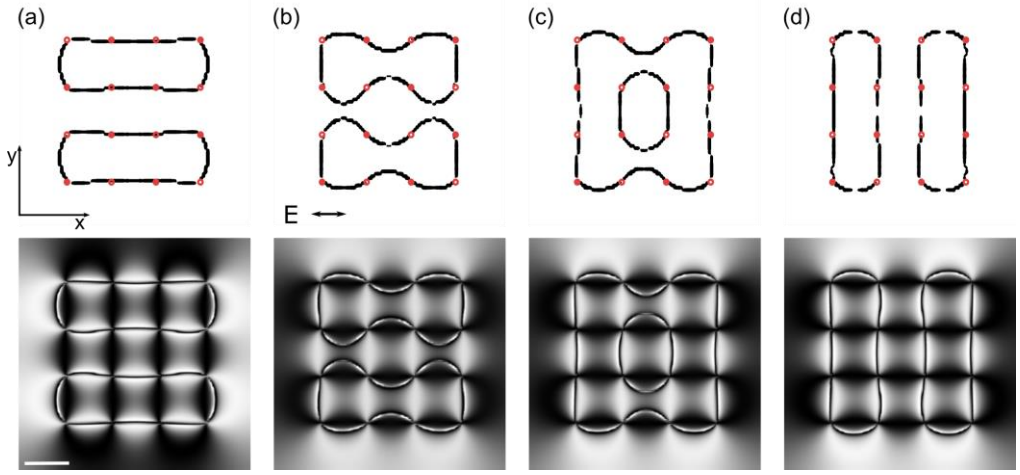

Figure 1: Numerical simulation of an electric field driven transition from a) the original configuration through (b, c) other configurations to a d) qualitatively the same structure as in a), except rotated. Top: red dots show locations of defects, enforced by the surface, black areas show lower ordering, indicating presence of defects. Bottom: simulated image under crossed polarizers.

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Environmental benefits of biomass pyrolysis and biochar production

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There is a need to increase the share of world energy demand (>400 EJ, 2017) met from renewable energy (18%, 2017). There is an existing and untapped potential for sustainable bioenergy production (270 EJ) [1]. Therefore, the European Commission has announced the "European Green Deal" to decarbonize energy-related sectors and become a climate neutral continent by 2050, as well as to protect and improve soil fertility and food quality [2]. Biomass pyrolysis has the potential to contribute, at least in part, to reducing global warming and enhancing conservation efforts.

Slow pyrolysis is a thermo-chemical conversion of biomass in the absence of oxygen at temperatures above 300°C and low heating rates. Unlike combustion, pyrolysis is a carbonization process in which only portions of the biomass are devolatilized, leaving much of the carbon in the form of char. If the biomass, the pyrolysis process and the char produced meet the criteria listed in the "European Biochar Certificate", the solid product can be labeled biochar [3]. In addition to biochar, gases and liquids are produced that can be burned to produce energy. Since biochar is not produced to be burned for energy, but is used in a way that preserves the carbon it contains, it should be noted that the energy yield of the pyrolysis process is about half that of combustion. Biochar is a stable material; therefore, pyrolysis is considered a carbon-negative technology and a viable pathway for long-term carbon sequestration to mitigate climate change. In addition, the properties of biochar, mainly related to its surface properties, make it a valuable soil amendment that affects soil fertility by increasing its ability to retain water and nutrients and to inhabit microorganisms.

Slovenia is almost 60% covered with forest. It ranks 4th in Europe and is among the top 30 countries worldwide. Over the past two decades, the Slovenian government has cut an average of about 3 million cubic meters of trees per year through regular (2/3) and sanitary (1/3) woodcutting. In 2014, a glaze ice disaster damaged more than half of Slovenia's forests. Due to the subsequent bark beetle infestation, 4 million cubic meters of trees were felled annually for sanitary reasons only. As a result, huge amounts of cheap wood (€25-50 per cubic meter) were collected, creating the possibility of producing economically feasible wood-based biochar with simultaneous bioenergy production. In this way, huge quantities of CO_2 would be removed from the atmosphere, leading to less global warming and preserving soil fertility, all in accordance with the principles of sustainability, circular economy and zero-waste policy.

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Mechanical, thermo-physiological and moisture management properties of flame-retardant textile screen-printed with $Al(OH)_3$ and cellulose nanofibrils

Tjaša Kolar[1], Vanja Kokol[1]

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Aluminium hydroxide nanoparticles (ATH NP) in a combination with phosphorylated nanocellulose (PCNF) have been used for treatment of fire retardant (FR) textile. Both nanomaterials were printed on fabric by conventional screen-printing process as nano-structured thin-layered coatings, to improve thermo-physiological comfort (moisture absorbency, good water vapour and heat transfer) without affecting its FR properties. Heat and water vapour transmission through fabric are two of the most important factors affecting the comfortable feeling when worn, since they control the transfer of excessive heat and water away from the body [1].

ATH NP with relatively high thermal stability (up to 500 °C) at lower loadings (<10%), were used as an energy-adsorbing [2] additive in a printing (polyacrylate)-paste (PaP) applied on a FR textile. In addition, PCNF was used as a renewable nanomaterial, acting as a dispersion media for ATH NP and simultaneously to improve the fabric moisture management. The printing was performed as one and two-layer coating to evaluate the effect of both printing strategies, where ATH NP were added either to PaP or PCNF.

As shown on Figure 1, the air permeability of fabric was reduced up to 45% by printing of PaP containing ATH NP and/or PCNF itself. However, the presence of ATH NP increased the fabric's mechanical properties up to 14% in warp direction, while lowered the water vapour resistance for 16% and thermal resistance for 17%. Such a treated fabric also retained up to 12% more of applied 21kW m-2 heat flow (simulating the temperature of 565 °C), and shift degradation temperatures for 15°C towards higher values (compared to reference sample).

ATH NP together with PCNF improve mechanical properties of the fabric as well as its functional properties: increase heat protection, increase water vapour and thermal transmissions, thus improving wearing comfort during heat exposure.

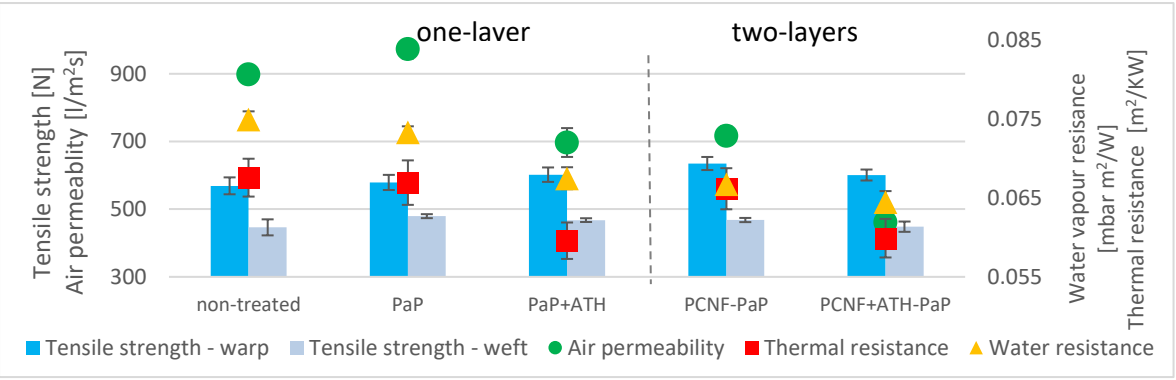

Figure 1. Functional properties of differently printed textile fabric

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Synthesis of magnetically responsive core-shell anisotropic magnetic nanoparticles coated with silica for magneto-mechanical actuation

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Anisotropic magnetic nanoparticles, such as nanoplatelets and nanochains, are gaining great interest due to their distinctive non-spherical shapes [1], [2]. Indeed, their tunable shapes and sizes allow new functionalities, such as magneto-mechanical actuation [3]. This technique is based on the remote manipulation of targeted soft matter with mechanical torque generated by moving anisotropic magnetic nanoparticles in a rotating or oscillating magnetic field at low frequencies. The exerted forces on soft matter that are in contact with the moving nanoparticles can lead to the rupture of cellular membranes, stimulate mechanoreceptors or induce structural changes in soft matter. The surface morphology of nanoparticles plays a key role in the contact interactions (adhesion) between nanoparticles and targeted soft matter. However, the role of surface morphology is still poorly understood and requires more investigation due to the challenges related with nanoparticle synthesis. The main reason for lack of data on magneto-mechanical effect is the challenging synthesis of nanoparticles with suitable dimensions and magnetic properties for medical uses as well as due to difficulties with well-defined surface coatings.

Here, we focused on procedures to synthesize silica coatings of different thicknesses and surface morphologies on magnetic nanochains and nanoplatelets. Smooth surface silica coatings were synthesized using standard Stöber procedure. To obtain rough mesoporous silica coatings, we utilized our own recently developed procedure based on soft templating [4]. We were able to produce diverse silica coatings on nanomaterials with different shapes and dimensions, as shown in Figure 1. We demonstrated protocols for thin and thick smooth coatings as well as silica coatings with tunable roughness.

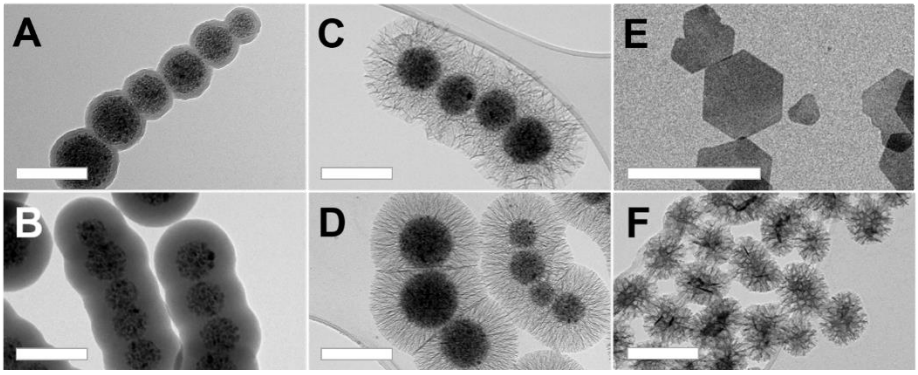

Figure 1: TEM micrographs of silica-coated anisotropic magnetic nanoparticles: nanochains with thin (A) and thick (B) smooth coatings, nanochains with different rough coatings (C, D), nanoplatelets with very thin smooth coating (E) and nanoplatelets with rough t

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Using the Ion S5 System for next-generation sequencing of Late Pleistocene and Holocene *Bison* samples

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During the last 130 ka there were two species of *Bison* present in Europe. The first was the steppe bison (*Bison priscus*), which appears in the European fossil record during the early Middle Pleistocene. It inhabited a territory from Western Europe, the Caucasus, the eastern coasts of the Black Sea and over large parts of Central and North Asia to North America. While the species became extinct in Europe at the end of the Late Pleistocene, it survived in parts of Asia and North America until the Holocene.

The extinction of *B. priscus* left the extant European bison or wisent (*Bison bonasus*) as the only *Bison* on the continent. *B. bonasus* is traditionally considered a Holocene species, as its morphologically distinct osteological remains first appear in the fossil record at the beginning of the Holocene, around 12-11.7 ka BP. However, cave art from France and Kazakhstan, as well as recent genetic analyses, suggest its existence or the existence of another, as yet undefined ancestral species as early as the Pleistocene.

Fossils belonging to both species have also been discovered in Slovenia and Hungary. Remains of the steppe bison have been discovered mainly in caves or quarries. In Slovenia, bones of the European bison have been found mostly in stilt-house settlements, and after the Chalcolithic no remains can be attributed to the species with certainty. In contrast, the species survived in Hungary up to the 18th century.

While the traditional classification of fossils is based on the use of their morphological characteristics and many of them are usually fragmented, new methods have been introduced in the last decades, such as the analysis of DNA, extracted from archaeological or palaeontological material (ancient DNA or aDNA). An invaluable tool in the analysis of ancient DNA is next-generation sequencing, due to its ability to sequence short fragments (<100bp).

In this study, we aim to develop and implement a simple methodology to amplify short fragments of the mitochondrial genome of ancient steppe bison and European bison from Slovenia and Hungary using the Ion S5 System (ThermoFisher). We intend to develop a metagenomic barcode-based approach using next-generation sequencing technology for the successful amplification of aDNA, extracted from Late Pleistocene and Holocene *Bison* bone samples. The barcode system is based on the amplification of short DNA segments tagged with an additional barcode sequence. This allows us to create a library by pooling and sequencing more fragments from a single sample in one chip run. We designed the primers to amply short fragments (106 bp to 198 bp) of the *Bison* mitochondrial genome.

PCR amplifications were performed on various Late Pleistocene and Holocene samples, targeting different regions of the mitogenome (12S, 16S, BND1, BND2, COX1, COX3, BND3, BND4, and cytochrome b). The methodology developed in this study will make a significant contribution to the analysis of bison aDNA using the Ion S5 System.

VaaMPIII-3: a disintegrin-like/cysteine-rich protein from the nose-horned viper venom and its effect on platelets

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Disintegrin-like/cysteine-rich proteins are haemostatically active toxins found in viperid venoms. Their antithrombotic action contributes to the haemorrhagic effect of the venom and helps the snakes to catch and digest their prey. These proteins consist of two non-catalytic domains and were originally interpreted as autoproteolytic products of the P-III class of snake venom metalloproteinases (SVMPs). However, a recently discovered disintegrin-like/cysteine-rich protein VaaMPIII-3 from the venom of the nose-horned viper (*Vipera ammodytes ammodytes, Vaa*) turned out to be a product of evolution, in which the gene encoding a P-III SVMP lost its entire metalloproteinase domain as well as part of its disintegrin-like domain. As such, VaaMPIII-3 defined a new subclass of SVMPs, termed P-IIIe, and raised the possibility that some other disintegrin-like/cysteine-rich proteins also have a similar origin.

The disintegrin-like domain harbours a highly conserved SECD motif that interacts with integrins on the surface of platelets and inhibits platelet activation and aggregation. This motif is also present in the truncated disintegrin-like domain of VaaMPIII-3. The cysteine-rich domain, which is intact in VaaMPIII-3, mediates interactions with plasma and extracellular matrix proteins. Our goal was to biochemically and functionally characterise VaaMPIII-3, the first member of the new P-IIIe subclass of SVMPs.

We isolated the protein from *Vaa* venom using several chromatographic techniques and determined its biochemical properties. We constructed a three-dimensional homology model of VaaMPIII-3 to predict some of its key structural properties. We tested its effect on human platelets and found that VaaMPIII-3 inhibited platelet aggregation with similar potency to other disintegrin-like/cysteine-rich proteins. It inhibited either ADP-, collagen- or arachidonic acid-induced platelet aggregation and thus qualified for use in the development of new antithrombotic drugs.

To further investigate the biological functions of VaaMPIII-3 and establish their structural determinants, we produced VaaMPIII-3 recombinantly in *E. coli* and evaluated its structural conformity and suitability for use in subsequent research. We will present our latest results, including a comparison of the biochemical properties of the natural and recombinant forms of VaaMPIII-3.

KAZALO AVTORJEV/AUTHOR INDEX

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Institut "Jožef Stefan" Ljubljana, Slovenija

Institute Jožef Stefan (IJS) is a research institute in Slovenia, which conducts a wide range of basic and applied research.

Mednarodna Podiplomska Šola Jožefa Stefana (MPŠ) provides postgraduate education in the fields of nanosciences and nanotechnologies, ecotechnologies, information and communication technologies, and sensor technologies.

NACIONALNI INŠTITUT ZA BIOLOGIJO
NATIONAL INSTITUTE OF BIOLOGY

The National Institute of Biology (NIB) is a basic, developmental and applicative research institution in the fields of biotechnology, biophysics, biomedicine and system biology.

CINKARNA

Cinkarna Celje, d.d., is a modern Slovenian chemical company that operates in accordance with the best available techniques and the principle of sustainable development.

SCAN

SCAN represents, sells and services products from world-renowned manufacturers in the field of electron microscopy, vacuum and cryotechnics.

Chemass d.o.o. is an authorized distributor for the sale and maintenance of instruments of the so-called "Life Science and Chemical Analysis" field of the manufacturer Agilent Technologies.

Sanolabor is the largest Slovenian company selling medical devices, laboratory equipment, medicines, personal protection products and dental products.

Pivovarna Laško Union (PLU) is the leading brewer and a highly competitive producer of cider and refreshing soft drinks in Slovenia.

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Student council 2020/2021: