10 - 11
May 2018

10th STUDENT CONFERENCE

Jožef Stefan International Postgraduate School
and Young Researchers'Day
(CMBE-Chemistry, Material, Biochemistry, Environment)
(Piran, Marine Biology Station - NIB)

NATIONAL INSTITUTE OF BIOLOGY

Institut
"Jožef Stefan"
Ljubljana, Slovenija

»Decoding Science:
Science Communication, Dissemination and Research«

Conference proceedings

Workshop on public presentation

Poster presentation

3-minute »Elevator Pitch«

Early April

Science
Technology
Engineering

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10. ŠTUDENTSKA KONFERENCA MEDNARODNE PODIPLOMSKE ŠOLE JOŽEFA STEFANA IN 12. DNEVA MLADIH RAZISKOVALCEV (KONFERENCA KMBO)

Zbornik

10th JOŽEF STEFAN INTERNATIONAL POSTGRADUATE SCHOOL STUDENTS CONFERENCE AND 12th YOUNG RESEARCHERS DAY

Proceedings

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Contents

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

Jeseni tega leta se bo vpisala na Mednarodno podiplomsko šolo Jožefa Stefana – MPŠ že petnajsta generacija podiplomskih študentov. Vpisujejo se praviloma najboljši iz Slovenije, pa tudi mnogi iz tujine, tako da so zmogljivosti šole praktično v celoti zasedene. MPŠ se je že uveljavila doma kot tudi v tujini, postala mednarodno prepoznavna, kar kaže, da je bila njena ustanovitev več kot upravičena. V vsem tem času je uspešno opravljala svoje poslanstvo, kar kažejo kvalitetna doktorska in magistrska dela. To je rezultat po eni stani uspešnega sodelovanja podiplomskih študentov in njihovih mentorjev, po drugi strani pa možnosti, ki jih nudijo ugledne raziskovalne institucije, ki v tem procesu sodelujejo. Na prvem mestu je treba omeniti Institut »Jožef Stefan«, ki največ doprinaša k uspešnemu delu te šole z odlično opremo vključno s centri odličnosti ter širokim izborom kvalitetnih mentorjev. Vključitev in sodelovanje Nacionalnega inštituta za biologijo – NIB in Inštituta za kovinske materiale in tehnologije – IMT je še razširilo naše potenciale in prispevalo k še večjim možnostim povezovanja in izkoriščanja razpoložljivih kapacitet interdisciplinarnosti. Moramo omeniti tudi podporo, ki jo naši šoli nudi gospodarstvo, zelo zaželena pa bi bila tudi večja podpora v obliki skupnih projektov.

MPŠ in navedene raziskovalne institucije so se in se zavedajo, da je ključnega pomena za uspešno delovanje v pogojih ekonomske in tehnološke globalizacije stalno spremljanje razvoja znanosti in inovativnosti v svetu. Na tem mestu moram omeniti nerazumno podfinanciranje znanosti s strani države, kar nedvomno prizadeva celotno visokošolsko znanstveno delovanje, indirektno pa tudi gospodarstvo. Pristali smo pri dnu EU držav s trenutno 0,36 % BDP državnih vlaganj v znanosti. Medtem ko že razvite države še naprej pospešujejo vlaganja v znanosti, manj razvite pa nas dohitevajo in prehitevajo, se v Sloveniji praktično ne dogaja nič oz. ostajamo le pri obljubah ali zavajanjih. To celo pri sedanji gospodarski rasti, ko pametni še pospešujejo vlaganja v raziskave in razvoj – R&R! Zato je razumljivo, da najrazvitejše države predstavljajo mladim raziskovalcem atraktivno delovno destinacijo kot tudi prostor za udobno življenje. Že samo glede na tako stanje težko enakopravno sodelujemo z razvitimi sredinami, čeprav v to vlagamo ogromno truda. Mednarodne povezave in globalizacija znanosti najbolj koristijo najrazvitejšim, kar pospešuje "beg možganov", ki smo mu priča tudi pri nas. Visokošolsko izobraževanje ter znanost pripadata danes generaciji brez meja! Danes je postala beseda "odličnost" izjemno popularna v svetu, zlasti na področju znanosti. Za odlično znanost pa morajo skrbeti izključno države same oz. njihove vlade! To razviti zelo dobro vedo. Pri različnih razpisih, še zlasti Obzorje 2020, so uspešni le tisti projekti, ki dobijo oceno odlično ali celo izvrstno. Osnovne raziskave s takimi ocenami naj bi vodile s svojimi prelomnimi dosežki do novih inovacij in proizvodov, od katerih je odvisna ekonomska rast in moč države. Slovenijo kot tudi mnoge manj razvite in nerazvite države tare predvsem nizka produktivnost. Rešitev tega problema je le v intenzivnih vlaganjih v raziskave in ljudi, kot je izpostavila januarja 2018 v Davosu Christine Lagarde, direktorica Mednarodnega monetarnega sklada – IMF. Zato pa je potrebnih veliko naporov in finančnih vlaganj vlad, ki razumejo pomen znanosti in raziskav za razvoj celotne družbe. Le tako bodo te države, tudi Slovenija, lahko uspešno vzpostavile sodelovanje z industrijo ter razvijale produktivne partnerske odnose. Za Slovenijo velja, da bi morala njena vlada vlagati čim prej vsaj 1 % BDP, če želi kolikor toliko nadoknaditi že zamujeno. Lep primer je Portugalska! Zmotno je mnenje, da bomo le s sredstvi EU dosegli želene

cilje. Ker že govorimo o odličnosti, smo pri projektih ERC odličnosti prav pri dnu EU. Glede na navedeno nas ne sme presenečati, da smo priče begu možganov in ne kroženju, kot to željo nekateri prikazovati.

Kljub vsemu naša MPŠ vlaga velike napore v doseganje več kot solidnih, v nekaterih primerih tudi odličnih rezultatov v sicer neprijaznih pogojih na področju raziskovalne in visokošolske dejavnosti. To kažejo objave v mednarodno uglednih in v nekaterih primerih vrhunskih revijah. Seveda teh uspehov ne bi bilo brez primerne infrastrukture ter odličnih mentorjev in somentorjev, ki so prejeli za svoje delo vrsto domačih ter mednarodnih priznanj. Naj omenim še izjemno vzdušje in kolegialne odnose, ki vladajo med podiplomci in njihovimi mentorji. Vse to omogoča kljub veliko vloženemu trudu kar uspešno vpetost v mednarodne povezave tako v evropskem kot tudi v globalnem prostoru. S svojim delovanjem MPŠ prispeva k hitrejšemu prehodu iz vsesplošne krize v družbo znanja. Tudi letošnja predstavitev raziskovalnih dosežkov naših podiplomcev je dokaz vaše uspešnosti, kar je posledica talenta in veselja do raziskovalnega dela. Vse to vam omogoča, da se boste ob pomoči mentorjev ter bližnjih sodelavcev razvili v kreativne raziskovalce, na katere bomo ponosni tako doma kot tudi v tujini. 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 odhodom v tujino. Vsekakor se je nujno potrebno bolj angažirati za boljšo prihodnost doma. Slovenija je lepa dežela, ni pa to samo po sebi dovolj!

Še enkrat bom ponovil, kar sem tudi že večkrat izjavil, da je "znanje vrednota, ki omogoča narodu ekonomski razvoj in obstoj". Zato postavimo končno znanost in znanje na tisto mesto, ki kulturnemu narodu pripada! Na prvem mestu so za to odgovorni politiki, ki so v zadnjih letih dokazali, kako malo cenijo znanje in tiste, ki ga ustvarjajo. Le od nas vseh je odvisno, do kdaj bo tako! Zato še enkrat ponavljam, da bi se morali mladi bolj angažirati, kot to počno vaši vrstniki v tujini. Mladi vrhunski raziskovalci so pogoj za uspešen gospodarski in vsesplošen razvoj in so srce družbe znanja. Očitno so za to spoznanje potrebne globoke družbene spremembe, ki pa jih do sedaj še nismo dočakali. Vendar bodimo še naprej optimisti.

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

Slogan letošnje študentske konference "Dekodiranje znanosti - pridite in se nam pridružite!" ponovno kaže na odprtost študentov MPŠ, ki želijo o znanstvenoraziskovalnem delu govoriti na način, ki bo razumljiv študentom in raziskovalcem različnih strok. To je predpogoj za dialog in ustvarjanje novih stikov in oblikovanje bodočega in odprtega sodelovanja. Izmenjava znanj in izkušenj med študenti in raziskovalci krepi in bogati raziskovalno delo, ki je po naravi večinoma interdisciplinarno. Letošnja konferenca nadaljuje s prakso prejšnjega leta, da je potrebno o znanosti govoriti na način, ki je razumljiv kar se da širokemu spektru ljudi. Take veščine so prirojene le redkim, zato je program konference posvečen tudi pridobivanju veščin javnega nastopanja.

Povezanost dveh tradicionalnih študenstkih konferenc; Študentske conference MPŠ in Dan mladih raziskovalcev kemije, biokemije, materialov in okolja (KMBO) na Institutu "Jožef Stefan" (IJS) se je v lanskem letu izkazala kot zelo uspešna, zato so se študentje tudi letos odločili za skupno delo in k temu pritegnili tudi študente zunaj IJS in MPŠ, kar je vsekakor uspeh organizatorjev konference in celotnega Študentskega sveta MPŠ, ki so konferenco promovirali na različne načine. Organizacija konference na nacionalnem Institutu za biologijo na Morski biološki postaji v Piranu, ki je pomemben partner MPŠ, pa bo omogočil širjenje povezav v zahodni del Slovenije.

V Sloveniji je vloga javnosti v znanstveni sferi pogosto zanemarjena, čeprav Evropa prepoznava, da je ta segment ključen pri prenosu znanja v prakso, zato je to zapisano tudi v strateških ciljih, kar se odraža v zahtevah tematskih razpisov Obzorja 2020. Tudi MPŠ prepoznava pomen komunikacije širši javnosti kot sestavni del izobraževalnega procesa, zato bo tovrstne dejavnosti še naprej podpirala.

V sodelovanju s partnerskimi raziskovalnimi institucijami in industrijo želimo na MPŠ ustvariti pogoje, ob katerih študentje lahko ustvarjajo odlično mednarodno primerljivo znanost, hkrati pa razvijajo svoje kreativne in poslovne sposobnosti, s čimer bodo prispevali tudi k zagotavljanju pogojev za uspešen razvoj poslovnih modelov in posledično k vidnim rezultatom v družbi. K temu vsekakor sodi tudi povezovanje programov MPŠ z ostalimi slovenskimi in tujimi univerzami, saj želimo študentom nuditi najboljše znanje in spretnosti, ki jih bodo v prihodnje rabili na svoji karierni poti.

Vsem udeležencem študentske konference želim uspešno delo, ki bo ostalo v spominu kot ustvarjalno in prijetno združenje.

Deans words, Prof. dr. Milena Horvat (eng)

The slogan of this year's student conference "Decoding science - Come and join us!" demonstrates the openness of IPS students who want to talk about scientific research work in a way that is understandable to students and researchers of different disciplines. This is a prerequisite for dialogue and the creation of new contacts and the formation of future and open cooperation. The exchange of knowledge and experience between students and researchers strengthens and enhances research work, which is by nature mostly interdisciplinary. This year's conference continues with the practice of the previous year that it is necessary to talk about science in a way that is understandable to a wide spectrum of people. Such skills are inherent in rare, so the conference program is also dedicated to acquiring the skills of communication to the public.

Joint organisation of two traditional student conferences; Students' IPS Conference and Young Researcher Day in Chemistry, Biochemistry, Materials and Environment (KMBO) at the Jožef Stefan Institute (JSI) proved to be very successful last year, and this year, students decided to work together again. Moreover, they decided to attract also students outside the JSI and IPS, which is definitely the success of the conference organizers and the entire IPS Student Council that promoted the conference in various ways. The organization of the conference at the National Institute of Biology at the Marine Biology Station in Piran, which is an important partner of the IPS, will enable the expansion of connections to students in the western part of Slovenia.

In Slovenia, the communicatioin of science results to the general public and other stakeholders is often neglected in the scientific sphere, although Europe recognizes that this segment is crucial in transferring knowledge into practice. This is why the need for effective communication and outreach activities are included in activities and the requirements of Horizon 2020 thematic calls. The IPS also recognizes the importance of thes eactivities as an integral part of the educational process, and will continue to support such activities in the future.

In cooperation with partner research institutions and industry, we want to create conditions at the IPS where students can create excellent international comparable science while developing their creative and business skills. Therefore, creating conditions that allow integration of IPS programs with other Slovenian and foreign universities, in order to provide the students with the best knowledge and skills they will need in the future on their career paths, is a logicall way to proceed in the future.

I wish all participants of the student conference a successful work that will remain in memory as a creative and pleasant gathering.

Izr. prof. dr. Matjaž Kuntner Direktor Nacionalnega Inštituta za Biologijo

Na Nacionalnem Inštitutu za Biologijo z veseljem gostimo študentsko konferenco Mednarodne podiplomske šole Jožefa Stefana. Zavedamo se pomena prenašanja vrhunskega znanja na mlajše generacije. Konference, kot je ta, so še posebej pomembne v slovenskem znanstvenem prostoru, ki je prostorsko, jezikovno, kulturno in tradicionalno precej omejen za širjenje znanja in kroženje idej. Znanost pa je v današnjem svetu izrazito globalna. Če nisi vpet v globalno znanost, kot znanstvenik ne obstajaš. Ključnega pomena za nove generacije podiplomskih študentov je, poleg spremljanja globalnih trendov, tudi kritično razmišljanje, česar se ne naučiš iz knjig, temveč iz interakcije znotraj generacije in med generacijami znanstevnikov. Prepričan sem, da se bodo na konferenci zaiskrila mnenja in porodile nove ideje. Nenazdanje je potrebna za znanstveni preboj tudi sproščena atmosfera. Podiplomski študenti, najdite jo na konferenci v Piranu!

"Decoding Science – Science Communication, Dissemination and Research"

Študentski svet

Letošnje leto smo že drugič uspešno združili dve uveljavljeni konferenci, in sicer študentsko konferenco Mednarodne podiplomske šole Jožefa Stefana (MPŠ) ter Dan mladih raziskovalcev kemije, materialov, biokemije in okolja (KMBO). Že lansko leto se je to izkazalo kot dobra ideja, saj sta obe konferenci namenjeni predstavitvam raziskovalnega dela podiplomskih študentov in sta večinoma potekali v zelo kratkem časovnem razmaku. Enako kot lani so se z združitvijo konferenc strinjali tako Odbor za konferenco KMBO kot tudi dekanja MPŠ, prof. dr. Milena Horvat.

Ker pa je letos študentska konferenca praznovala 10. jubilej, smo organizatorji prestavili prostor dogajanja izven Ljubljane. Lokacija konference je tako postala Piran, njena organizacija pa je potekala v sodelovanju z Nacionalnim inštitutom za biologijo in Morsko biološko postajo Piran. Organizacija konference je v primerjavi s prejšnjim letom predstavljala veliko večji zalogaj, saj smo poleg same priprave predstavitvenega in znanstvenega dela morali poskrbeti tudi za prevoz in prenočitve. Navkljub oddaljenosti konference izven glavnega mesta pa smo prejeli 49 prispevkov, katerih avtorji so svoje znanstvene dosežke predstavili tako z »elevator pitch« predavanjem kot tudi s posterjem.

Očitno je konferenca zanimiva tudi za vrsto podjetij, saj smo finančno podporo prejeli s strani kar štirih podjetij (Scan, VWR, Primatron in Eppendorf). Prav tako pa so nam podjetja priskrbela tudi promocijski material (Kemomed, Mikro Polo) ter poskrbela za snemanje predstavitev študentov (Videolectures). Ves čas pa so nam pri organizaciji stali ob strani sodelavci tajništva MPŠ in njeni profesorji, brez katerih ne bi uspeli izvesti konference na takšnem nivoju.

Konferenca je potekala dva dni, v tem času so vsi študenti z oddanimi povzetki predstavili svoje raziskovalno delo s kratko tri minutno predstavitvijo, imenovano tudi »elevator pitch«, ter s predstavitvijo plakata. Strokovna komisija je predstavitve in plakate ocenila ter podelila štiri nagrade najboljšim udeležencem, najboljšega kandidata pa je med vsemi izbrala tudi publika. Svojo nagrado pa je podelil tudi projekt ISO-FOOD, ki deluje v okviru Odseka za znanosti o okolju na Institutu »Jožef Stefan«. Med predstavitvami so svoj del odpredavali tudi trije vabljeni predavatelji, kjer je vsak od njih predstavil komunikacijo znanosti z drugačnega vidika. Igor E. Bergant je predstavil komuniciranje znanosti z vidika novinarja, kakšne pasti se skrivajo v komunikacijski vrzeli med novinarjem in raziskovalcem ter kako le-te premostiti. Kako naj bi raziskovalec komuniciral s stanovskimi kolegi, je v svoji predstavitvi prikazal prof. dr. Matevž Dular s Strojne fakultete UL, ki je lansko leto prejel financiranje s strani Evropskega raziskovalnega sveta za utrjevanje samostojne raziskovalne poti (ERC Consolidator Grant). Podajanje informacij oziroma komuniciranje o znanosti z javnostjo pa je v svojem govoru predstavil Mišel Cevzar, eden od lanskoletnih zmagovalcev konference MPŠ in sovoditelj podkasta Meta PHoDcast.

Namen konference je poleg predstavitve raziskovalnega dela podiplomskih študentov bilo tudi medsebojno povezovanje, izmenjava idej, predlogov in kritik ter sklepanje novih poznanstev in partnerstev med vsemi obiskovalci. Kajti le s povezovanjem različnih vej znanosti in seveda znanstvenikov lahko upamo na boljšo prihodnost.

"Decoding Science – Science Communication, Dissemination and Research"

Student council

This is the second year during which the two conferences – the Student Conference of the International Postgraduate School of Jožef Stefan (IPS) and the Day of the Young Researchers of Chemistry, Materials, Biochemistry and Environment (CMBE) – have been combined in a single event. It was evident from last year that combining the two conferences is a good idea, since both of them were targeting more or less the same audience and they were organised over a very short time span. Just like in the previous year, the idea of combining the two conferences found approval with both the CMBE Organising Committee and the dean of the IPS, prof. dr. Milena Horvat.

Since this was the tenth consecutive year during which the student conference was organised, the organisers decided to move the conference away from Ljubljana to Piran, with the help of the National Institute of Biology and the Morska biološka postaja Piran (Marine Biology Station Piran). The organisation of the conference proved to be a bigger task, compared to last year, since, besides the preparations for the presenting and the scientific part of the conference, we also had to take care of the transportation and the accommodation. Despite the remoteness of the conference, we received 49 abstracts, the authors of which presented their scientific achievements as an "elevator pitch" as well as a poster.

The conference was also interesting for a number of companies, and we received financial support from them (Scan, VWR, Primatron and Eppendorf). Also, the companies provided us with promotional material (Kemomed, Mikro Polo), and took care of recording the student presentations (Videolectures). Throughout the organisation of the conference, the staff of the IPS secretariat and the IPS professors offered us great support and without them we would not be able to hold a conference at such a level.

The conference was held for two days, during which time all of the students with submitted abstracts presented their research work in a short, 3-minute presentation called an elevator pitch, as well as the presentation of a poster. The expert commission assessed the presentations and posters and presented four awards to the winners. The audience also picked their own favourite presenter and another prize was awarded by the ISO-FOOD project, which is being run by the Department of Environmental Science at the Jožef Stefan Institute. Three invited lecturers also had presentations, each of them presenting the topic of science communication from a different perspective. Igor E. Bergant presented the communication of science from the viewpoint of a journalist, explaining the traps that are hidden in the communication gap between the journalist and the researcher and how to bridge them. How a researcher should communicate with his or her colleagues during a presentation was described by prof. dr. Matevž Dular from the Faculty of Mechanical Engineering UL, who received an ERC Consolidator Grant last year. Presenting information or communicating about science with the general public was presented by Mišel Cevzar, one of the last year's winners at the IPS conference and a co-leader of the podcast Meta PHoDcast.

In addition to presenting the research work of postgraduate students, the purpose of the conference was to interconnect, exchange ideas, develop proposals and make constructive criticism, and to make new acquaintances and partnerships. It is only by combining the various branches of science and, of course, scientists that we can hope for a brighter future.

Ekotehnologija (Ecotechnology)

Tritium dispersion around Krško Nuclear Power Plant

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The population of Slovenia, like population elsewhere in the world, is exposed to natural ionizing radiation, as well as to certain anthropogenic sources of ionizing radiation, which come primarily from the use of such radiation in medicine, the Chernobyl contamination and the contamination generated by atmospheric nuclear tests. When it comes to residents in the surroundings of the Krško Nuclear Power Plant (NPP), we could add the release of atmospheric radioactive substances [1].

Since H-3, Sr-90 and Cs-137 are part of the global contamination, they are present everywhere on Earth's surface and we cannot directly prove their origin. Moreover, surveys show that concentration of such radionuclide as Cs-137 in surroundings of Krško NPP are likely the result of Chornobyl disaster and/or nuclear tests but not the operation of Krško NPP. As for now, tritium is practically the only radionuclide that can be attributed partly to the releases from the Krško NPP [1].

Tritium is a beta emitting radioactive isotope of hydrogen with half-life time of 12.6 y. Tritium is formed by the interaction of the atmosphere with cosmic rays. Also, it could be formed as a result of nuclear reaction in NPPs and nuclear testing. As tritium has slight difference in physical and chemical characteristics in comparison with H-1, it can be exchanged with hydrogen atoms in environmental water. So, the tritium is involved into the hydrological cycle, and can enter the human body by inhalation and ingestion [2].

The aim of this research was to obtain first results of airborne tritium in the surroundings of Krško NPP, and based on those measurement results to compare them with the existing atmospheric dispersion model including the dose estimate for the representative person [3].

Results of research show good agreement between measured and modeled results and their ratios are within from 0.6 to 2.7.

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Discrete AlF_4^- Fluoroaluminate Anion in the Structure of [IPrH][AlF_4]

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Aluminium forms very strong complexes with fluoride, thus making AlF_3 the most thermodynamically stable compound with extremely high lattice energy.[1] Consequently, AlF_3 and similar fluoroaluminate species preferentially adopt the octahedral coordination of aluminium. Typically, AlF_n units in such materials form ionic crystal structures with arrays of cations and anions which are assembled into a myriad of connectivities.[2] Furthermore, according to the literature, several multinuclear complexes of fluoroaluminate anions and discrete hexafluoroaluminates have been prepared and structurally characterised. On the other hand, crystallographic data for discrete fluoroaluminate anions are still limited, because of difficulties related to the growth of single crystals.[3] Up to date, only a few compounds of tetrahedral coordinated fluoroaluminates have been found.

Our research focused on the synthesis of new fluoroaluminate complexes. During our work, we managed to prepare a discrete tetrahedrally coordinated AlF_4^- anion and to characterise it by X-ray crystallography of single crystal of [$IPrH^+$][AlF_4^-] (IPrH+ = 1,3-(2,6.diisopropylphenyl)-imidazolium ion) (Figure 1).

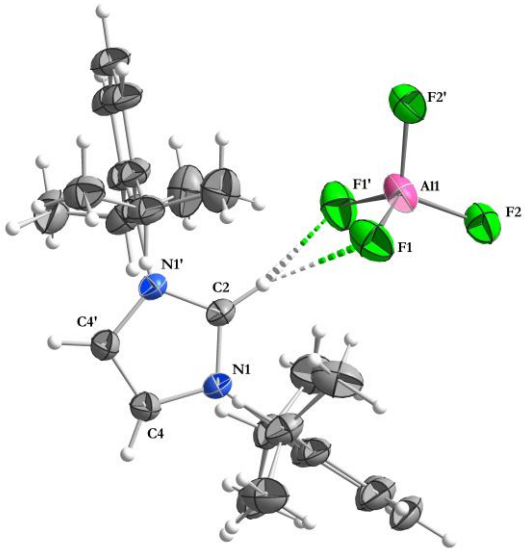

Figure 1: The asymmetric unit of [$IPrH^+$][AlF_4^-]. Thermal ellipsoids are given at 30 % probability level.

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CONTROL OF CELL BEHAVIOUR THROUGH DEVELOPMENT OF ALIVE BACTERIA-POLYELECTROLYTE COMPOSITES

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Modifying surface charge of the bacterial cells can tremendous increase their biotechnological potential since this can affect the process of attachment to different surfaces, can induce formation of homo- or heterocellular aggregates, enables attachment of enzymes for faster start-up of bioreactor processes and others. Since bacterial cells resemble negative surface charge mainly due to the negatively charged phospholipids, it has been shown to be convenient for polyelectrolyte deposition on their surfaces. Nevertheless, complexity of the structure of the surface of the cell, cell size and weight, division rate and properties of the extracellular macromolecular layers produced by the cell complicate relatively straightforward methods of polyelectrolyte deposition. Moreover, since bacterial cell is not as simple as inorganic particle, surface lining of bacterial cells, comprised of membrane and cell wall, is also involved in respiration as well as transportation of different molecules, which additionally complicate process of surface modification. For effective coating of alive bacterial cells, on one hand it is important to prepare the most efficient method based on physicochemical principles and on other hand, it is needed to have in mind the physiology of the particular type of bacteria.

Therefore, our aims were to determine: (i) the interference of the growth stage of the culture on the efficiency of deposition of polyelectrolytes on the surface of the individual alive bacterial cells and (ii) the response of the bacterial cells after the polyelectrolyte nano-sized layers were formed on their surfaces.

According to our results, bacterial cells entrapped in polyelectrolyte shells showed delayed growth and slower division rate. The delay of the bacterial growth resulted from the mechanical restriction of individual cells, since we did not observe any kind of toxic effect on the *Escherichia coli*. Moreover, here we also proved that such modified cells showed tremendous ability to attach to different sorts of surfaces. By increasing their stickiness, we were also able to control intercellular interactions between different cells as well as guiding them to the particular site.

Development of the analytical procedure for the determination of polybrominated diphenyl ethers in human serum by gas chromatography – inductively coupled plasma mass spectrometry

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Polybrominated diphenyl ethers (PBDEs) are a group of persistent organic pollutants that were added to many commonly used products such as textiles, polyurethane foam, plastics, mobile phones, television sets, computers and construction materials for the purpose of reducing their inherent flammability. Since PBDEs are not covalently bound to the matrix of consumer products, they are susceptible for leaching into terrestrial and aquatic environment where they have a tendency to bind to organic fraction of particulate matter, soils and sediments. Their hydrophobicity and resistance to degradation enables them to bioaccumulate and biomagnify in living organisms, including humans. To assess exposure of humans to PBDEs, a new simple, reliable and sensitive method was developed for the determination of six PBDE congeners (BDE 28, BDE 47, BDE 99, BDE 100, BDE 153, BDE 154) in human serum by GC-ICP-MS. PBDEs were extracted from 1 mL of serum by 30 minutes of mechanical shaking with formic acid. Afterwards, 2 mL of iso-octane was added and 30 minutes of mechanical shaking applied. Co-extracted lipids were removed by a rapid and low solvent consuming clean-up step using Florisil column, which is much more straightforward compared to existing cleaning procedures that are laborious and require large amounts of organic solvents. The analytical method was validated by analysis of standard reference materials NIST SRM 1957 and 1958. Good agreement of determined concentrations with those certified was found. Repeatability and reproducibility of analytical method was within 5.9% and 6.1%, respectively, while limits of detection (LODs) for the PBDEs analyzed were between 0.0016 and 0.0039 ng mL^{-1}. Feasibility of the method was tested by analysing six real human serum samples. Determined concentrations in sera from this work were in the same range as those reported for some other European countries. BDE 47 was most common as it was detected in all samples analysed. BDE 99 and BDE 100 were also quite frequent. The highest concentration found was for BDE 153 (0.0145 ng mL^{-1}), which was not that abundant in other samples analyzed. Due to its simplicity, sensitivity, reliability and low amount of sample needed for the analysis, the method will be used in the future work for the purpose of biomonitoring.

The impact of 'radon-based stability' on aerosol particle pollution at Ljubljana Basin

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Radon (^{222}Rn) is a naturally occurring radioactive gas permanently exhaling from the ground into the atmosphere. Being noble gas, it is transported by turbulent diffusion without chemical reactions or deposition, and it is unlikely to be washed out by rainfall. The only significant sink of radon is radioactive decay. Therefore, it is able carry geophysical information over long distances across Earth's crust, oceans and atmosphere. Daily variations of radon activity concentration in the atmosphere is related to daily changes in the lower atmosphere vertical mixing state (or "atmospheric stability"). Recently, atmospheric radon has been used as an alternative method to assess atmospheric stability. The atmospheric stability is expressed by several categories, playing an important role in estimating the magnitude and time evolution of pollutants, among which nano particles are significant.

The complex landscape of the Ljubljana with generally calm winds exhibits frequent persistent cold-air pool. Thus, in autumn and winter months, in stable atmospheric conditions, it is subject to relatively large aerosol particle pollution. The aims of the study were: (i) development of atmospheric stability classification scheme based on hourly measurements of atmospheric radon (named 'radon-based stability', with the following categories: weakly unstable (1), neutral (2), weakly stable (3), moderate stable (4), strongly stable (5)) and (ii) the implementation of 'radon-based stability' classification on measured nano particle data, mean total number concentration C_{tot}^{N} of ultrafine (<100 nm) and fine (<1000 nm) particles.

Measurements of radon and nano particles in outdoor air have been conducted in the Ljubljana. Radon has been continuously monitored, using an AlphaGuard radon monitor (Saphymo, Germany). Nano particles in the size range 10–1100 nm have been measured continuously for several days on November 2017 with an Aerosol SMPS+C instrument, Series 5.400 (Grimm, Germany), about 4 m above the ground.

The highest C_{tot}^{N} of ultrafine particles have been observed during the morning and evening rush traffic hours (range: 6655−26,686 cm^{-3}). While C_{tot}^{N} of fine particles have been distributed throughout the day with an increasing concentration during the afternoon (range: 1645−16,734 cm^{-3}). Good correlation has been found between the C_{tot}^{N} of ultrafine and fine particles and 'radon-based stability' classification. The more stable is the atmosphere, the higher is nano particle pollution. Consequently, the C_{tot}^{N} of ultrafine and fine particles under strongly stable category have been found to increase by a factor of 5 and 2, respectively.

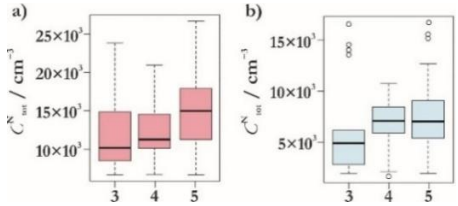

Fig.1. Box and whisker plots C_{tot}^{N} for a) of ultrafine particles and b) of fine particles, under three categories of 'radon-based stability' (3: Weakly Stable, 4: Moderate Stable and 5: Strongly Stable).

Study of the stability and fate of BPA and its alternatives during water treatment

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Bisphenol A (BPA) and its alternatives (BPs) are industrial chemicals used in the production of polycarbonate plastic, epoxy resins and thermal paper. Since BPs are structurally similar to BPA, a known endocrine disrupting compound, they have the potential to exert similar toxic effects once they enter humans and/or the aqueous environment.

To assure accurate results, the stability of selected 18 BPs was checked in methanol (MeOH), wastewater (WW) and MilliQ-water. Their stability was evaluated based on chemical analysis by gas chromatography-mass spectrometry (GC-MS). Samples were spiked with the target compounds (20 μg L^{-1}) and stored in the dark at a − 20, 4 and 25 °C and 0, 1, 4, 12 and 24 week time intervals. In addition, the removal efficiency of different water treatments, namely bench-scale suspended and attached growth bioreactors and direct UV light photoreactors was studied. The bioreactors were operated under identical conditions in terms of hydraulic retention time (HRT: 48 h), a working volume (4 L) and synthetic WW compositions. Influents and effluents were sampled for half a year with monthly intervals. Photo-treatment was performed in a cylindrical glass reactor by exposing 760 mL of an aqueous solution of BPs in Milli-Q water to direct UV irradiation for 10, 20, 40, 60, 120 and 240 min. The concentrations for both treatments were chosen based on the typical levels of BPs in real WW reported in the literature (BPs: 200 ng L^{-1} and BPA: 1 μg L^{-1}).

The experimental design enabled an evaluation of the influence that the matrix, temperature and time have on the stability of BPs. The results reveal no significant drop in concentration for BPs stored in MeOH, while in the case of WW and MilliQ-water, storage time exerted an influence factor on BPs stability. After 4 weeks, the BPs, with the exception of BPM, BPP, BPPH, BPBP and BPFL, remained stable (concentration drop < 20 %). Biological treatment resulted in the high removal (> 80 %) of the majority of the BPs, where no significant difference between the suspended and attached growth biomass was observed. In the preliminary test, where adsorption onto sludge was estimated, the results suggest that this process contributes considerably to the overall removal of certain BPs (e.g. > 90 % for BPF and BPE). Degradation of the BPs under UV-treatment followed pseudo-first-order kinetics. The kinetic profiles and removal efficiency differs among the studied BPs (removal = 0 – 73 %) after 2h of UV irradiation. To our knowledge, this is the first study of the stability, biodegradation and photodegradation of 18 BPs, which can support the reliable assessment of the fate of BPs in the environment.

Generation of a test dataset for machine learning–assisted identification of contaminants of emerging concern

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The ever increasing number of environmental contaminants of emerging concern (CECs) requires employment of sophisticated analytical techniques for the purpose of their identification and quantification through non-target analysis. One of them is gas chromatography coupled to mass spectrometry (GC-MS), a robust technique that demands derivatization of semi-polar contaminants to improve their volatility and thermal stability. Among most commonly used derivatization reactions is trimethylsilylation, i.e. addition of a trimethylsilyl (TMS) group, which improves the chromatographic behaviour of a compound, but also affects its fragmentation resulting in an MS fingerprint completely different from that of the underivatized compound. MS library search is the straightforward approach for compound identification, but, due to the lack of GC-MS and GC-MS/MS spectra of TMS derivatives, a more powerful identification strategy is needed. None of the state-of-art computational tools deals with *in silico* compound identification based on the EI-MS(/MS) spectra of TMS derivatives. Therefore, we target this gap by developing an input-output kernel regression (IOKR)-based machine learning tool. The first step towards reliable machine learning-supported compound identification consisted of cautious generation of test and training datasets. Namely, the model has to be trained and tested on datasets containing appropriate number of compounds with specific substructure signatures, MS fingerprints and MS/MS spectra, which offer both sufficient structural and chemical diversity within each dataset and differences between datasets, therefore ensuring unbiased identification performance.

The purpose of our study is to generate training dataset of MS and MS/MS spectra of TMS derivatives of CECs with proper specificity, authenticity and quality. The 23 CECs analysed thus far include 5 estrogen hormones, 5 non-steroidal anti-inflammatory drugs (NSAIDs), 7 parabens and 6 natural cannabinoids. All of them are derivatized with two derivatization agents, N-methyl-N-(trimethylsilyl) trifluoroacetamide (MSTFA) and N, O-bis(trimethylsilyl)trifluoroacetamide (BSTFA) under experimental conditions optimized using design of experiments (DOE). The derivatives were analysed using GC coupled to each of the three mass analyzers: mass selective detector (MSD), ion trap (IT) and triple quadrupole analyzer (QqQ). So far we have generated 69 MS and 138 MS/MS spectra of the 23 TMS derivatives of CECs.

In order to enhance the reliability of the test dataset, our further work includes evaluation the specificity and quality of the acquired MS and MS/MS spectra by determining the distribution and the acceptable variability of spectral peak intensity at each m/z value along the analyzed mass range and fragment ion: isotope intensity ratios. By selecting 7 to 10 statistically significant group- and compound-specific fragment ions, with intensities varying within the confidence interval (95%), we aim to ensure proper development and performance evaluation of the IOKR tool, and hence reliable compound identification when applied to non-target environmental analysis.

Determination of uranium isotope ratios by MC-ICP-MS

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Precise and accurately determined uranium isotope ratios are essential for geochronological dating and tracing of different environmental processes. In addition, they are of paramount importance for nuclear safeguards and nuclear forensics.
Multi-collector inductively coupled plasma mass spectrometry (MC-ICP-MS) has become an important tool for determination of isotopic composition of uranium isotopes in various sample matrices. Its features are better accuracy compared to alpha spectrometry, which is comparable to thermal ionization mass spectrometry while maintaining higher sample throughput. This makes it an ideal tool for many applications.

The objective of this study was to develop, validate and verify an accurate analytical method for the determination of uranium isotope ratios ($^{235}U/^{238}U$ and $^{234}U/^{238}U$) with correctly estimated measurement uncertainty and apply them to real environmental samples.

Different approaches of sample preparation were tested to evaluate possible influence on uranium fractionation by trying various possible uranium pre-concentration (evaporation, co-precipitation with $Fe(OH)_3$, $Ca_3(PO_4)_2$ and MnO_2) and separation techniques (extraction chromatography, ion exchange chromatography and solvent extraction). Measurements were carried out with Nu plasma II, (Nu instruments Ltd, UK) MC-ICP-MS with the high-efficiency sample introduction system Aridus II™ (Cetac Technologies, NE, USA). At first, routine optimization and calibration of the MC-ICP-MS was performed. Then the concentration of purified uranium solution introduced to the MC-ICP-MS was optimized in terms of precision. Instrument mass bias was corrected with external standard – sample – standard bracketing technique.
The most optimal analytical procedure for precise determination of uranium isotopic composition in low concentrations was chosen to proceed on samples.

The developed method was applied on water samples of karstic aquifer (Ljubljanica catchment) to determine $^{235}U/^{238}U$ and $^{234}U/^{238}U$ ratios on MC-ICP-MS. The exact concentration of uranium in sample was determined by two different methods, by radiochemical neutron activation analysis (RNAA) and by inductively coupled plasma mass spectrometry (ICP-MS). The comparison of this two different methods was also performed.

Characterization of Spirulina algae as a new alternative food source

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Growth of world population and consequent increases in food production, losses in agricultural productivity and sustainable production methods are the reasons for production of alternative food products [1; 2]. *Arthrospira* is a cyanobacteria whose production requires lower water consumption and smaller land area compared to other agricultural crops, on product nutrient content basis. *Arthrospira* cell mass doubles in 4 to 5 days without the use of biocides and with low energy consumption [3]. As a good source of proteins, vitamins, fatty acids (FA), minerals and other nutrients, it is a good alternative food source that contributes to human health. *Arthrospira* products are sold in the market as Spirulina and are among leading dietary supplements [4]. For our research we gathered 46 samples of Spirulina products from the market in powder, tablet and capsule form. The aim of the research was firstly to analyse Spirulina FA content, as some authors reported the presence of long-chain polyunsaturated FA (gamma-linoleic, α-linolenic, eicosapentaenoic (EPA) and docosahexaenoic (DHA)) and omega-6 to omega-3 FA ratio to be 4 : 1 or less in Spirulina products. Secondly, we analysed Spirulina elemental composition, as it has been determined in previous research to be a good source of iron, calcium, phosphorus and magnesium. Lastly, the research consisted of stable isotope ratio analysis. Elemental composition and isotope ratio analysis were used to classify Spirulina products according to their geographical origin. To our knowledge, no research was done in this field on Spirulina up to now. Little research was done on quality analysis of the Spirulina products on the market, and no research in quality analysis of Spirulina products available on the Slovenian market. Our first results show a very low content of omega-3 FA and no EPA and DHA content in Spirulina products. However, high omega-6 FA content, including linoleic and gamma-linolenic FA was determined, rejecting the claims of 4 : 1 omega-6 to omega-3 FA ratio in these products. Results of the elemental composition analysis show high iron and cadmium content in our Spirulina samples. These newly discovered elevated Cd levels strongly decrease nutritional values of Spirulina and present a severe threat for human health. According to elemental composition, we managed to classify samples originating from Hawaii, resemblance has also been found among the samples from China and Taiwan and among samples from Mongolia. Future research using Fourier-Transform Infra-Red spectroscopy is planned to determine authenticity and Inductively Coupled Plasma Mass Spectrometry to further evaluate cadmium levels in Spirulina samples.

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Optimisation of the method for Sr isolation from the matrix for reliable determination of $^{87}Sr/^{86}Sr$ isotope ratio by MC-ICP-MS in milk

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The authentication and verification of the geographical origin of food commodities are important topics in the food sector. Over the last 6 years an increasing number of studies have been published covering the use of strontium (Sr) isotopes in distinct areas of food studies [1]. Swoboda *et al.* (2007) demonstrated that the Sr isotope ratios are less affected by seasonal variations during a year than other elements like hydrogen (H) and oxygen (O). Different $^{87}Sr/^{86}Sr$ isotopic ratios, reflecting only the variations in the amount of radiogenic ^{87}Sr present in the sample, depend on the age and on the pedological characteristics of soils where they naturally occur, namely their geographical origin. The result is that the Sr isotopic composition of a sample yields information about provenance, unobscured by local climate variations or biological processes [3].

The Sr has four stable, naturally occuring isotopes (^{84}Sr, ^{86}Sr, ^{87}Sr and ^{88}Sr). Only ^{87}Sr is radiogenic and its concentration gradually increases in minerals as a result of the β – decay of the rubidium (^{87}Rb) isotope. Due to isobaric overlap of ^{87}Rb with ^{87}Sr, Rb has to be removed from the sample prior to analysis by mass spectrometry. For separation of Rb and Sr, different separation methods may be used.

In general, the analytical method for $^{87}Sr/^{86}Sr$ ratio determination consists of several steps from sample pretreatment, separation of Sr from the matrix and measurement of the isotopic composition, where isolation of Sr from the matrix is the major challenge. Therefore, the aim of the study was the optimisation of the Sr isolation method from the milk. For the optimisation of the method, dehydrated milk sample (Pomurske mlekarne) was used. Milk is a complex matrix, which, besides water, contain a great variety of components, inorganic as well as organic. In order to achieve the effective separation of Sr from impurities and interferences, the organic matter must first be eliminated by complete oxidation. Two methods were checked as pretreatment procedures: dry ashing and microwave-assisted digestion. Further, Sr was separated from matrix impurities and potentially interfering elements using columns filled with Eichrom Sr specific resin. The efficiency of the extraction chromatography was determined by the determination for Sr concentrations in the eluent by inductively coupled plasma – mass spectrometry (ICP-MS). Extraction efficiences between 86 and 97% were obtained for all samples, regardless of the pretreatment method used.

In the next step, the isotopic composition of Sr will be determined by multicollector ICP-MS in order to exclude any isotope fractionation during the sample preparation step.

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Characterization of Slovenian apple and strawberry aromas for authenticity assessment using stable isotope approach

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It has been reported that synthetic flavours are sometimes sold as natural ones. At the moment, gas chromatography isotope ratio mass spectrometry (GC-C-IRMS) is perhaps one of the most specific and sophisticated method for determining food authenticity. For authenticity assessment of aroma compounds, several steps need to be taken including sample and standard selection, sample preparation, compound identification, $\delta^{13}C$ measurements, data processing, database creation. The authenticity of the aroma compounds can then be verified by comparison of the $\delta^{13}C$ value of the analysed sample with the values from a created database. The established protocols and methods were used in our study to investigate natural and commercially available apple and strawberry recovery aromas.

GC-MS identification analysis results of laboratory produced and commercial apple and strawberry recovery aromas show a difference in the presence or absence of certain aromatic components as well as the relationships between them. Commercial samples have more uniform composition compared to laboratory samples obtained, where variability is due to the different apple varieties. However further analysis is required for better understanding the meaning of presence or absence of certain aroma compounds. Since a rather small amount of components contributes to apple and strawberry aroma, we decided to investigate active aromatic components, which are also possible to be detected with GC-C-IRMS. For such analysis the selection of reference material and appropriate processing and interpretation of the results obtained is crucial. For this purpose, samples of pure synthetic aroma compounds have been first analysed on EA-IRMS and compared with literature data where we observed good agreement. One of the main objectives of the present research was to establish the database of $\delta^{13}C$ values for several most common flavour compounds present in apple and strawberry recovery aromas. Analysis of commercial recovery aromas, labelled as natural, revealed that the $\delta^{13}C$ value of the majority of the compounds present was within the expected authentic range. The data also revealed some possible falsifications of mainly strawberry samples. Our data also reveals some differences in $\delta^{13}C$ value between natural apple and strawberry recovery aromas, which requires further investigation. Although the method was developed to differentiate between natural and synthetic apple and strawberry aroma compounds it can be easily transferred also to other commodities. Research is implemented in the framework of SPS: Food for Future.

Molecularly imprinted polymers as solid phase extraction sorbents for the determination of sertraline and its analogues in aqueous matrices

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Our goal is to develop an analytical method for the determination of sertraline and its analogues found in environmental waters using molecularly imprinted polymers (MIPs), known for their high selectivity and affinity for their targets, as solid phase extraction sorbents. The presence of sertraline and its metabolite norsertraline in surface and wastewaters has already been confirmed[1,2]. Furthermore, our laboratory simulation experiment of irradiation of the parent drug also suggested the formation of norsertraline, sertraline ketone, sertraline imine and two hydroxylated analogues during exposure to sunlight.

The MIPs and their non-imprinted analogues (NIPs) for the antidepressant sertraline were synthetized by bulk thermal radical polymerization. After the polymerization the MIPs and NIPs were washed using Soxhlet extraction in 10 % acetic acid in methanol until no sertraline was detected in the washing solution. The rebinding properties of the synthetized MIPs were evaluated using batch rebinding experiments in different ratios of water and acetonitrile and comparing them to the corresponding NIPs. The determination of the sertraline concentration in the samples was analysed with high performance liquid chromatography coupled with a UV detector. The MIPs with the highest capacity and selectivity were ground, sieved and packed into SPE cartridges for additional evaluation. The compositions of the two MIPs with the best rebinding characteristics for sertraline were: methacrylic acid (MAA) as the functional monomer with ethylene glycol dimethacrylate (EGDMA) as cross-linker in chloroform, and a co-polymer of MAA and methyl methacrylate (mMA) with EGDMA in acetonitrile. The ratios between the template, monomer and cross-linker were 1/4/20 for the first, and 1/4/8/12 in the second synthesized MIP. 2,2'-azobis(2,4-dimethyl valeronitrile) was the initiator added in both cases. MIPs were additionally characterized by Fourier transform infrared spectroscopy and the particle size was confirmed by optical microscopy. Our next step is evaluating the rebinding characteristics of MIPs for the other sertraline analogues.

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Uptake of airborne fluorides by vegetation growing near pollution source

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Fluorine (F) is one of several trace elements receiving much attention owing to its possible harmful effects. In addition to naturals sources of fluorides (volcanoes, forest firing, oceans), different types of industrial activities contribute to the emission of gaseous and particulate fluorides into the atmosphere. For instance, hydrofluoric acid is used in the glass industry for etching, cleaning and making opal glass. During the processing of the glass at high temperatures some of the fluoride (F^-) is released.

Periods of higher than normal emissions occur in most industries due to human error, equipment failure or even combination of both. An accidental release of fluorides from industrial facilities can have severe consequences, because of F^- toxicity to humans, flora and fauna. Gaseous fluorides can travel significant distances downwind and can directly attack vegetation causing necrosis or tip burns (Fig. 1).

The present study was initiated by an appearance of necrotic lesions of vegetation typical for fluoride intoxication in the surrounding of glassworks factory Steklarna Rogaška. The aim was to establish if the cause was sudden, uncontrolled release of gaseous fluorides from the glass factory. The representative samples of damaged vegetation were collected, F was determined by fluoride ion selective electrode after preceding total sample decomposition and the pattern of F dispersion was suggested. The contents of F in vegetation exceeded the maximum levels of F for the complete feed for cattle, sheep and goats as recommended by the European Union standards and yielded a linear log-log fit with respect to the distance from the emitter.

Figure 1: Necrosis of spruce needles

Informacijske in komunikacijske tehnologije (Information and Communication Technologies)

Blood pressure prediction using data mining algorithms

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Hypotension (low blood pressure) and especially hypertension (high blood pressure) are heart diseases of global health concern. Chronic exposure to these medical conditions can gradually damage the entire body and often results in weak and rapid pulse, heart attack, kidney failure and other serious life-treating diseases. To improve the treatment, it's crucially important to monitor the blood pressure on a regular basis. In this research, our goal is to develop models that give an approximate estimate of the blood pressure in real time using data collected from sensors. Blood pressure readings are given by two numbers, i.e., systolic blood pressure over diastolic blood pressure measured in millimeters of mercury (mmHg). The difference between systolic and diastolic blood pressure is called pulse pressure. From a data mining point of view, we have a multi-target regression problem with three continuous target features: systolic, diastolic and pulse blood pressure. For building the models, we use two different approaches. In the first approach, we create a separate model for each target, while in the second we simultaneously predict the three target variables.

The data employed contains 21 features in total. Three of them are target features, while the rest are descriptive features. The dataset contains 1,429 data points. Each data point represents one measurement for a given patient, and there are multiple measurements per patient. The data contains measurements from 96 different patients. The descriptive features can be split in two groups, static and dynamic features. Static features are those that do not change across different measurements for the same person (e.g., sex, height, arm length), or are unlikely to change in a period of several weeks/months (e.g., weight). Dynamic features can and do have different values across different measurements (e.g., pulse wave velocity, heart rate).

Most of the effort in this project has been directed toward using data mining techniques to obtain predictions for blood pressure. We used several regression methods for single target prediction, i.e., linear regression, gradient boosting of regression trees, bagging of model trees and bagging of regression trees. Additionally, we used bagging of random subspaces with model trees as base learner for both single and multi-target prediction. Since we are interested in measuring the magnitude of the error, and errors in both directions (predicted blood pressure is lower or higher than the actual) have the same importance, we chose mean absolute error (MAE) as the most suitable performance metric. For evaluating the performance of the models, we use the leave-one-patient-out approach, where all measurements for a single patient are used as a test set.

After evaluating the constructed models, we conclude that gradient boosting of regression trees performs best. Second best is bagging of random subspaces using model trees. The MAE difference between the models built with those two algorithms is less than 0.3 mmHg. In the future, we will retrain the models on new data and try alternative experimental designs, with the aim of further improving the predictive performance of the models.

Neurodegenerative Diseases Data Ontology

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In this work, we propose the Neurodegenerative Diseases Data Ontology (NDDO), as a mid-level ontology for representing various types of data on patients with neurodegenerative diseases. The proposed ontology can be used for semantic annotation of datasets that contain different diagnostic data (clinical, imaging, biomarker, etc.) about neurodegenerative diseases and its progression, collected on patients by the hospitals. Having an ontology for describing data on patients with neurodegenerative diseases is important from two different perspectives: (1) from a viewpoint of ontology-based data access (ODBA) it would allow federation queries; (2) from viewpoint of data analytics it would allow (semi) automatic creation of data analysis workflows based on the datatypes that occur in the datasets.

The proposed ontology was constructed following best practices from ontology engineering. This involved the use of a top level ontology (Information Artifact Ontology) as a template, and a set of standard relations. We heavily reused classes and identified mappings to domain terms that are defined in previously developed biomedical ontologies and vocabularies available at BioPortal. This included terms from ontologies covering general medicine, neuroscience, and neurodegenerative diseases.

The ontology was constructed in a hybrid fashion. For this purpose, we used two instances of datasets on patients with neurodegenerative diseases, originating from two well-known studies concerning neurodegenerative diseases: Alzheimer's Disease Neuroimaging Initiative (ADNI) and Parkinson's Progression Markers Initiative (PPMI). We also used the domain terms that appear in documentation of ADNI and PPMI studies (study objectives, study protocols, study procedures, schedule of activities and others). To address the data analytics perspective, we also reused and extended our previously developed ontology of data types (OntoDT) and ontology of core data mining entities (OntoDM-core) to represent specific datatypes that appear in the domain of neurodegenerative diseases. The ontology construction and semantic annotation of the two instances of neurodegenerative diseases datasets was performed using semantic web technologies (RDF, OWL, RDFS), which are currently a popular solution to data and knowledge sharing and integration. For semantic annotation, we used Cellfie, a Protégé plugin which allows annotation of data stored in an Excel sheet. The mapping of the columns in the Excel sheet with the corresponding ontology classes was done through rules and axioms written in a Domain Specific Language based on Manchester OWL Syntax. Once we generated the annotations of each column, we used them to generate annotated data examples, which represent each row, i.e. instance of the dataset. However, this approach proved to be computationally expensive, as it makes the annotation even more challenging when working with larger datasets.

In the future, we plan to align the proposed ontology with the Ontology for General Medical Science (OGMS), Neurological Disease Ontology (ND), Phenotype and Trait Ontology (PATO), and NeuroPsychological Testing Ontology (NPT) in order to enable interoperability with already developed ontology resources in the domain of neurodegenerative diseases.

Acknowledgments: The data used in this work was obtained from the Alzheimer's Disease Neuroimaging Initiative (ADNI) and Parkinson's Progression Markers Initiative (PPMI). We also acknowledge the European Commission's support through the H2020 Human Brain Project SGA1 (Grant No. 720270) and the Slovene Human Resources Development and Scholarship Fund.

Classification of stellar types based on RAVE stellar spectra morphology

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The Radial Velocity Experiment (RAVE) survey is one of the biggest large scale spectroscopy surveys up to date, carried out using the 6dF multi-fibre spectroscopic facility at the UK Schmidt telescope. In this project we used data derived from the latest, i.e., fifth batch of RAVE data released, in order to determine one of the 12 possible stellar classes from data describing the stellar spectra, which contain many peculiarities characterizing each stellar type. Our training set consists of 4942 instances described by 1522 numerical attributes, 1500 of which are the intensities at different wavelengths in the spectra, 19 of them are linear integrals along with 3 colour magnitudes.

There are several challenges that need to be tackled when working with this data, which is highly unbalanced, starting with the pre-processing phase, all the way to the choice of the algorithm for predicting the stellar class. Given the three types of features (wavelengths, integrals and magnitudes), we generated three different datasets, in addition to the original dataset. First, we selected the wavelengths and colour magnitudes as descriptive attributes. The second dataset consists of only the linear integrals and colour magnitudes. Finally, the third dataset is a result of dimensionality reduction via principal component analysis (PCA). We have done PCA on the 1500 wavelength features by selecting the components that preserve 95% of the variance that these features carry. In addition to the feature selection, we address the imbalance of the data with several approaches, striving to obtain a balanced dataset. One of the approaches we used for addressing this problem is SMOTE (Synthetic Minority Over-sampling Technique), developed by Chawla et al. in 2002. We also apply an under-sampling technique and compare the two techniques on the pre-processed data.

The data obtained through these steps was used to train two types of ensembles of classification trees, i.e., Random Forests, and Ensembles of Bagged Trees. The ensembles included from 100 up to 500 trees. The comparison between the two types of ensembles was made for the ensemble sizes that produced the best scores for each ensemble type. In this project, we used the Matthews Correlation Coefficient (MCC) as the evaluation metric, which takes into account every member of the confusion matrix. Hence, for a highly imbalanced multiclass dataset like the one we use, it gives equal emphasis between the minority and majority classes. We estimated the performance of the models by using 10 fold cross-validation. The results show that the dataset with reduced dimensionality via PCA, containing 181 features, sampled with the SMOTE method using Random Forests as the ensemble method with 100 trees has higher Matthews Correlation Coefficient across all of the classes than the default dataset containing all 1522 features, with the default distribution, and Random Forest with 100 trees as the ensemble method which had the second highest MCC score. In the future, we will modify the sampling methods used before, while we will also build Ensembles of Boosted Trees as one possible solution for building better models.

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Meta learning for multi target regression

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In this work, we propose to address the problem of algorithm selection and hyper parameter optimization for multi target regression problems (MTR). Opposite of the mainly considered problem of a single target regression, where the interest is on a single variable, in MTR scenarios the output is a data structure – a tuple/vector of continuous variables. Many real-life tasks can be addressed with MTR, such as predicting the abundance of different species living in the same habitat, predicting properties of forests, energy efficiency of buildings. protein inhibition potential of chemicals, predicting behaviour, motor, cognitive scores for patients with neurodegenerative diseases etc. [1], 2].

For obtaining the top performance, a wide range of algorithms covering many different fields from machine learning to solving hard computational problems, require either choosing the right algorithm (known as algorithm selection (AS) problem) or tuning the right parameters (often treated as a special case of the AS problem). In machine learning literature, the problem of algorithm selection mainly evolved under the hood on what is known as meta learning. The importance of meta learning problem is providing a solution for automatic choice of machine learning algorithms. This can bring a chance for non-experts to successfully apply machine learning in their day to day activities. The basic principle behind meta learning is forming an abstract system for learning, aiming to optimize a performance measure, for new data on unknown problem. The core issue is to extract meta knowledge and generalize it from many different problems. Later, the obtained knowledge should be applied on new problems.

The focus on this work is on generating meta knowledge for regression problems in the form of meta features extracted from 33 multi target datasets. The various meta features/measures can then be used to describe the available datasets and use the descriptions to learn a meta predictive model. Several types of meta features have been proposed in literature and they can be categorized into three groups. In general, there are two approaches for generating the meta features. The first approach learns the complexity of a response surface via adapting meta features tested on single target problems – considering the global representation of the MTR problem. The idea is to capture the correlations between the feature and targets, the correlation between targets, input and output distribution and similar features [3]. The second approach employs meta knowledge that is shown to be successful for single target benchmark problems available at UCI repository. The obtained meta features will then be coupled with the estimates of the performance of 24 methods for multi-target regression thus yielding the meta dataset. We will then use predictive clustering trees for the multi-target regression and ensembles thereof [2] to learn the meta models. The single tree models will elucidate the potential knowledge conveyed with the features, while the ensembles will exploit to the fullest the information made available by the features thus obtaining the best predictive performance.

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Improving the efficiency of algorithms for developing complex rules in DEX methodology

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DEX (Decision EXpert) is a qualitative multi-criteria decision-modelling methodology. The models in DEX are used to evaluate and analyse decision alternatives. DEX models are composed of hierarchically structured attributes, their scales and decision rules. Scales are a small set of verbal values. Decision rules are assigned to aggregated attributes; for each aggregated attribute in the model, decision rules define a bottom-up mapping from subordinate to their parent attributes. Decision rules are represented in terms of a decision table, which maps all the combinations of subordinate attribute values to the value of the corresponding aggregated attribute. Each row in the decision table is called an elementary rule, which maps a particular value-vector to a single or interval decision value of the aggregated attribute.

Decision tables may contain many decision rules and may collectively be difficult to understand for the user. In order to obtain a more comprehensible representation, DEX-rule is an algorithm that converts elementary rules into more compact complex rules. Complex rules are areas limited by bounds which may cover more than one elementary rule and map to a single decision value. The DEX-rule algorithm generally works well, but was found inefficient in decision tables involving many (e.g., more than five) arguments and containing large areas that map to a single decision value.

This research was aimed at improving the efficiency of the DEX-rule algorithm. We proposed a novel algorithm, called jRule, and compared it with DEX-rule algorithm on selected examples of decision tables. The DEX-rule tries to find areas of elementary rules starting from one elementary rule and extending it in various directions. Consequently, the time complexity of this algorithm is $O(m^n)$, where m and n are the number of attributes and elementary rules, respectively. The main idea of jRule is to reverse the search and begin with the largest areas. When the search does not succeed, these areas are gradually reduced. As it turns out, the complexity is reduced to $O(n^2m)$. The two algorithms in general produce different complex rules, therefore we also compared them in terms of the number of created complex rules.

The experimental comparison of algorithms on two decision tables (Table 1) revealed that: (1) jRule's running times are significantly lower than those of the DEX-rule, and (2) the number of complex rules generated by jRule is usually lower.

	Running time [s]		Number of complex rules	
Examples	DEX-rule	jRule	DEX-rule	jRule
1	0.75	0.20	30	18
2	1280.0	0.395	121	64

Table 1: Difference between the two algorithms based on running time and number of generated complex rules (Both algorithms were compiled with same compiler and run on the same computer).

Towards end-to-end learning from heterogeneous networks

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Complex networks are becoming ubiquitous to modelling real life phenomena such as traffic, metabolism and community formation. Simple networks, which can be directed, undirected, weighted or unweighted are termed homogeneous networks. A complex network with additional properties assigned to nodes and edges is termed a heterogeneous network. We developed a novel end-to-end approach for learning from such networks.

The main task we address is node classification. Here, a subset of nodes in a network is labelled. The labels can for example represent different protein functions, types of users or different part-of-speech tags. The goal is to build a classifier P, which given a set of unlabelled nodes N_u and a set of labelled nodes predicts most probable labels L. The proposed approach builds on previous in-house developed framework for heterogeneous network decomposition HINMINE. Let M represent a heterogeneous network. A homogeneous network is a projection of the heterogeneous network, where relations between different types of nodes and edges are aggregated into edge weights between a set of labelled nodes. We propose a novel type of aggregation, where first all possible combinations of triplets {A,B,C} are taken into account. Here, nodes A and C are labelled and B is an intermediary node of a different type. Next, a heuristic function f : {A,B,C} → w needs to be specified. The w represents a real number and is in this work inspired by text mining heuristics such as the well known TFIDF. Applying a heuristic over occurrences of all possible triplets yields the final weight, assigned to an edge in the final homogeneous network.

As multiple heuristics $H=\{h_1,..,h_n\}$ are known for network decomposition, we determine the best heuristic by minimizing the error function E: $\{L, L_{real}\} \rightarrow Re$,

$$h_{opt} = ArgMin_{h \in H}\left[E\left(P\left(H\left(M\right), N_u\right), L_{real}\right)\right] \quad (1)$$

The P used In experiments is a simple logistic regression. We demonstrate, that using automatically constructed decomposition triplets yields similar or better results compared to manually chosen triplets. Finally, we formulate network decomposition as an optimization problem, solved over the space of all available heuristics. The optimization is implemented via a simple grid search procedure, where all heuristics are considered. Finally, triplets' weights are computed in parallel, which results in ~15% speedup compared to the original HINMINE decomposition routine.

Digital security in microfinance institutions

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The purpose of this paper is to present research proposal for PhD dissertation in awareness, benefits and challenges of digital security (DS). The target audience are microfinance non-banking financial institutions (MFI). The countries where the research would be conducted are Republic of Macedonia, Greece, Bosna and Hercegovina, Serbia and Albania[1] (selected countries). The expected contributions are measurement the level of awareness and vulnerabilities, attacks and risks for digital security in MFI. In addition to forecast the management of security, privacy and personal data protection risks in easy and affordable way.

The literature review was applied for identifying the requirements and the needs for digital security. IT strategies, policies and procedures have essential role for implementing DS. Also, training and digital education are extrapolated from the literature. Further analyses will be performed for cyber insurance for MFI.

We propose a methodology for examining DS, as mix of self-respond questionnaires and interviews with executives responsible for digital security. The structure of questionnaire will be based on interviews with 3 MFI. Ethical issues are recognized during all process of the study. (starting with access, data collection, data storage and interpretation of results). The study will not have "sensitive personal data". Written consent will not be obligatory for participants.

Potential benefit will be guides for better protected MFI in the digital single market. Also, increased interest of MFI to become active players when implementing General data protection regulation (GDPR). Finally, reduced economic damage caused by harmful cyber attracts. (privacy incidents and/or data protection breaches). The main outcome is to determine whether different practitioners will be enable to share responsibility along all actors (micro clients, MFI and regulators) for digital security in the selected countries. However, it will be crucial to identify whether the need for better business or regulatory requirements are the key trigger for implementing appropriate digital security.

Keywords: microfinance institution, digital security

[1] Selected countries would be further determinate

The impact of feature selection on the performance of link quality estimation

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There are many parameters that can affect wireless communication links. Some of them can be influenced by engineers, for instance the radio hardware characteristics, operation frequency, bandwidth, modulation and protocols. Others are due to the natural environment such as the weather condition, interference (constructive/destructive), background noise and obstacles. One way of describing the state of the wireless links at different points in time is by using link quality estimators.

To date, there are a number of link quality estimators proposed in the literature. Some of them use hardware metrics such as LQI, RSSI and SNR, others use software metrics such as PRR and RNP. The estimators also differ in their approach of gathering relevant metrics. They can be *active* by sending probes in the network, *passive* by only using observed or received data, or *hybrid* which is a combination of the two. The estimators also differ depending on where they operate, on the *receiver*, *transmitter* or *both* sides). The typical link quality estimators are manually built by developing a model that fits measure data. More recently, several researchers have proposed automatic methods for developing link quality estimators using adaptive machine learning algorithms.

While existing work has shown that the input metrics influence the performance of link quality estimators, it is unclear what metrics are best used and why.

In this paper, we propose a systematic study on the influence of feature selection on the performance of machine learning based link quality estimators. Our study considers first order features, up to fourth degree polynomial features and quantiles. We will be using R^2 (R-squared) as a criteria, along with F-test and mutual information, in search of how a particular feature may explain future Packet Reception Ratio (PRR) changes. The most promising subset features will finally be tested on a set 4 different classifiers (i.e. logistic regression, decision trees, random forest and SVMs) and a set of 4 regression algorithms (i.e. linear regression, lasso, multi-layer perceptron and simple neural network).

Identification of a Nonlinear Dynamical Benchmark System using Process-Based Modeling

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Many applications in a variety of domains consider modeling of real-world systems, where almost each system is nonlinear and dynamical. Suitable models are to achieve highly accurate reconstruction, and are often used for prediction of an observed system's behavior under diverse conditions.

Process-based modeling is a grey-box modeling approach, joining knowledge-driven (white-box) and data-driven (black-box) modeling approaches, simultaneously identifying the structure of the model and estimating its parameters. This formalism allows for automated discovery of quantitative laws and models, expressed as equations, from measured data and domain-specific knowledge. The resulting process-based model offers both high-level explanatory representation of a dynamical system in terms of its principle system components, as well as their transformation into a low-level formalism in terms of equations adequate for simulation of the system's behavior.

Mechanical oscillating processes constitute an important set of nonlinear dynamic systems. Real-world examples are the suspensions in motor vehicles, where shock absorbers and progressive springs are important components. In this work, we tackle the task of reconstructing a well-known benchmark in the domain of system identification, i.e. a nonlinear mechanical oscillating system, called the Silverbox system, which can be seen as an electronic implementation of the Duffing oscillator. The data available for this system is generated by an electrical circuit close to idealized representation of the oscillator. The equation describing this system's behavior relates the displacement y(t) (the output) to the force u(t) (the input).

$$m\frac{d^2y(t)}{dt^2} + d\,\frac{dy(t)}{dt} + k\big(y(t)\big)y(t) = u(t)$$

The parameter *m* is a moving mass, *d* is viscous damping, and *k(y)* is a nonlinear progressive spring described by a static but position-dependent stiffness with the following equation:

$$k\big(y(t)\big) = a + b\,y^2(t)$$

The task of obtaining a process-based model of this particular system starts with defining the search space of all plausible model structures, i.e. creating a library of background knowledge, where we define template entities with which we represent the oscillator (and its parameters) and template processes that describe its behavior in the form of equations. In order to limit the space of model alternatives, incomplete model structure is introduced as modeling presumption, where we point which particular templates to be used in the model structure. We obtain a list of all enumerated (and feasible) candidate model structures, for each of which the task of parameter estimation is executed with the use of measured data. The output consists of a list of complete process-based model structures, ranked according to their performance measured on the training data. The simulations obtained from the best model structure is highly comparable the train data, from which we can conclude that our process-based model is a quality reconstruction of the Silverbox system. To this end, this process-based model can be used for precise prediction of this particular system's behavior.

A Semi – Automatic Approach for Borrowing Missing Nutrient Values in Food Composition Databases

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Food composition data (FCD) are detailed sets of information on the nutritional components of foods, provide values for energy and nutrients, food classifiers and descriptors and are presented in Food Composition Databases (FCDBs). The data contained in currently available FCDBs is of differing quality which depends on the data source. Analytical data is the most trustable and accurate, and FCDBs can be used more confidently when the values are known to be based on original analytical values. Two of the main limitations of FCDBs are: variability in the composition of foods between countries and incomplete coverage of foods or nutrients leading to missing data. Major problem in FCDBs are missing values of components, which must never be assigned a zero value, and which distort the integrity of the database. Therefore, good quality FCDBs should aim towards minimizing the number of missing data. The most used approach for resolving missing data is borrowing data from tables and databases from other countries where a reference back to the original source may or may not be possible.

According to the current rules or rather suggestions for borrowing FCD, the FCDB used for borrowing should contain the foods and nutrients of interest and/or be produced from a country that is similar in geographic location. However, this technique can be very inaccurate. To the best of our knowledge a semi – automatic approach for borrowing compositional data between countries does not exist. For this reason, we propose such an approach for borrowing missing nutrient values. It uses modelling based on null-hypothesis testing, where the end result for a missing value of a specific nutrient in a food from a given country is a value obtained from a set of countries whose FCDBs are eligible for borrowing.

Using EuroFIR FCDBs and the proposed methodology we crate rules for several European countries for specific foods. For example, if in the Italian FCDB for raw beef meat there are missing nutrients then these values can be calculated based on the values from the same food from the FCDBs of: the UK, Switzerland, Sweden, Denmark, USA, Canada, Slovenia and Finland but the value from the FCDB of the Netherlands cannot be included in the calculation. The methodology is evaluated using leave-one-out-cross-validation, and the end results of above mentioned example shows that using our methodology in 87.86% gives better results than the regular calculation for borrowing.

As the preliminary results of the presented study are promising, this methodology can be further extended on more countries and more foods and evaluated using leave-one-out-cross-validation. Ideally rules will be generated for all foods and all nutrients.

Physical activity, nutrition and mood monitoring for health coaching

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Lifestyle choices can strongly influence our health and well-being. Important factors that can be easily improved are nutrition and physical activity. Our tasks in the context of health coaching application are activity recognition, nutrition monitoring and mood assessment. Understanding person's mood can help give advice at the appropriate time, which is important for a successful behavioural change.

Using classical machine learning methods, we have developed a model that can classify emotions from speech audio signal. We trained a feedforward neural network with a feature set for emotion recognition and achieved accuracy of 81%. We will further improve this result using deep neural networks. We can estimate the mood of the recommendation system's users by checking their emotions periodically, when they engage with it using a natural language interface. Mood estimation can be improved using nutritional and activity data, such as time of meals and amount of physical activity, which have been shown to influence mood.

Physical activities of interest are different types of exercise (e.g., walking, running, cycling) and activities of daily living (e.g., chores, personal hygiene, rest, food preparation). Nutrition monitoring will consist of recognizing food-related activities (food preparation, eating). We have merged two different datasets containing measurements from wrist worn sensors. By extracting features from accelerometers we have achieved 86% classification accuracy for 6 classes (running, rest, walking, nordic walking, rest, handwork) and 70% accuracy with additional class for eating. We expect to improve models by adding additional features to classify wrist motion better. Consequently, more nutrition-related activities could be recognized. Possibly some further improvement could be achieved by merging more databases.

Further work will be a study of correlations between activity recognition, nutrition monitoring and mood assessment. We will investigate questions such as how does a change of mood affect the users' nutrition habits and physical activity, as well as the other way around. The findings will improve the understanding of health behaviours, interaction of mood, nutrition and activity, and facilitate the development of behaviour change interventions, since simple recommendations are often not enough to adopt healthier behaviours.

Elbow assistance exoskeleton to facilitate high level control design

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Exoskeletons devices are a wearable technology that is making rapid progress and has progressed to the point where the devices can provide assistance in periodic tasks like walking and running. Many current advancements rely on advanced control algorithms, however, the mechanical design is just as important. We can learn from the human body which is adapted for walking on uneven terrain or performing tasks in unstructured environments. Its specialized actuation, i.e. muscles and their architectures around joints, are an important reason why such feats are possible and why the human body still outperforms the current best humanoid robots.

The group of novel actuators, called mechanically compliant actuators, transfer some of the human body capabilities to humanoid robots or wearable devices. These actuators employ, besides a main geared motor, an additional elastic element built into a mechanism. Additionally, it is equipped with a second, smaller motor. Such configuration can adapt and be compliant when collisions are expected or more rigid when precision is desired. Additionally, the compliant element can store elastic energy, enabling more efficient movements and allow the approximation of external forces without the heavy load cells. The technology is suitable for exoskeleton actuation since exoskeleton devices work in synchrony with the human and must be very adaptable. While the increased number of components raises the design complexity, weight and cost, on the other hand, it opens many possibilities for design simplification.

Our experimental exoskeleton (Fig. 1 and 2) employs a novel variant of such a compliant actuator (Fig. 3). Its architecture combines a cam and a variable lever mechanism in a rotational structure and results in a pseudo-linear torque deflection characteristic and in a compact design. Due to the perpendicular stiffness variation, its second motor can be small and of low power, which further decreases the weight and energy consumption. The exoskeleton and its unique actuation we designed in combination with different sensors, will provide us with the means to study high level exoskeleton control algorithms like the neural networks, deep learning, etc.

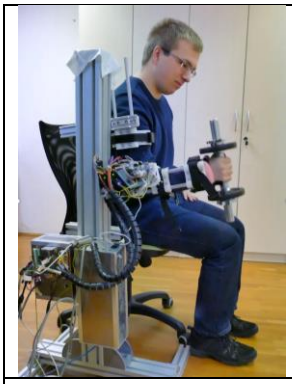

Figure 1: Exoskeleton prototype

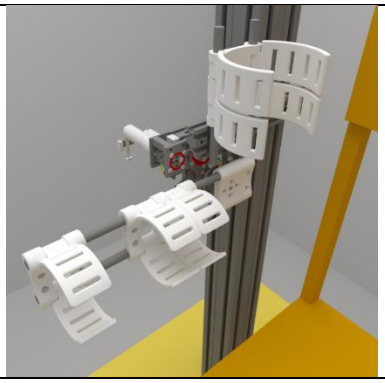

Figure 2: Exoskeleton model

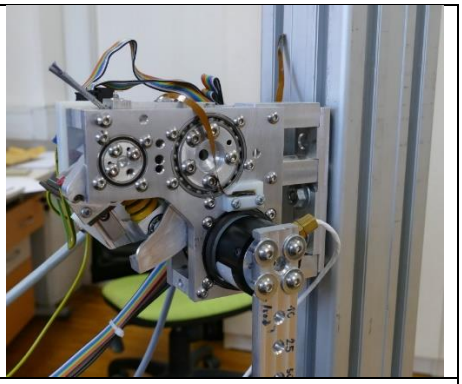

Figure 3: Actuator prototype

Nanoznanosti in nanotehnologije (Nanosciences and Nanotechnologies)

Anisotropic nanocrystalline Nd-Fe-B magnets produced by spark plasma sintering

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Green technology is an important issue in the direction of preserving and maintaining sustainable environment via wind turbines, electric vehicles and electric generators [1]. For such applications, Nd-Fe-B magnets are the most suitable choice due to their high energy product $(BH)_{max}$. The larges $(BH)_{max}$ value of 433 kJ/m^3 was reported for high-performance anisotropic hot-deformed (HD) Nd-Fe-B magnets [2]. However, the coercivity needs to be improved in order to withstand the demagnetization fields during motor operation. Adding heavy rare earths (HRE) such as Dy or/and Tb, results in the formation of high anisotropy (HRE, $Nd)_2Fe_{14}B$ phase which leads to the enhanced coercivity. The drawbacks of using HRE are reduced magnetic saturation, price and risk of supply since they are predominantly mined in China [1]. Therefore, high performance Nd-Fe-B magnets with a reduced amount of HRE or even without HRE needs to be considered.

There are several options to produce hot-deformed magnets, and one of them is spark plasma sintering (SPS) process. By SPS, the production of magnets at low temperatures and short times is possible. This is necessary to hinder the grain growth, which would cause the reduced coercivity and with SPS we can avoid this [3].

Hot-deformed magnets are prepared in two stages. In the first step, the hot-pressed magnet (at 675 °C, 1 min, 3.9 kN, vacuum) was prepared from melt-spun ribbons to achieve fully dense magnet (Fig. 1 (b)). In the second step, the hot-pressed magnet was plastically deformed (at 700 °C, 1 min, 7.2 kN, vacuum) at higher pressure, which results in the anisotropic alignment of $Nd_2Fe_{14}B$ grains along the pressing directions (Fig.1 (c)). Strong alignment of the $Nd_2Fe_{14}B$ grains leads to higher remanence and lower coercivity. 10 % improvement of the coercivity was achieved after the post heat treatment at 600 °C for 60 min.

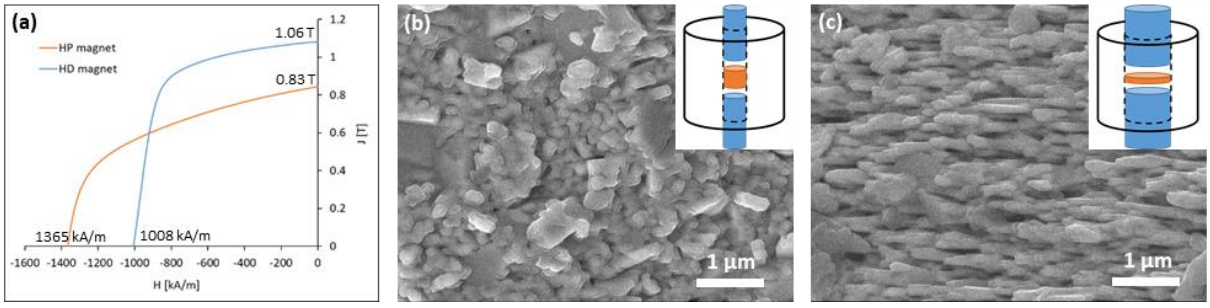

Figure 1: (a) Demagnetization curves of hot-pressed (HP) and hot-deformed magnets (HD), (b) SEM image of HP magnet and (c) SEM image of HD magnet.

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Topological defects in smectic ordering

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In this work we present topological defects in smectic–A liquid crystal. We focus on edge dislocations which appear due to bend imposed deformations. We describe the phenomenological model of smectic–A liquid crystals to study the topological defects of our interest. We introduce the free energy of the smectic A liquid crystal and we compare it to the description of superconductors, emphasizing similarities. It is well known that in superconductors of type-II topological defects could be stabilized. Type-II superconductors are characterized by a large enough ratio between the magnetic penetration length λ and the order parameter correlation length. We derive expressions for analogous lengths in smectic–A liquid crystal. Based on them we determine the regime where edge dislocations could be stable if a bend elastic distortion is imposed to smectic–A liquid crystal. Furthermore, some preliminary experimental results, obtained by means of polarizing optical microscopy and high-resolution calorimetry, in mixtures of the chiral liquid crystal CE8 compound with gold nanoparticles will be presented.

Hybrid Silane Acrylate Coating for Corrosion Protection

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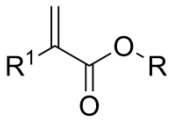
Epoxy coatings have been one of the most widely used forms of protection of steels against corrosion. No major alternative appeared in the last years which could replace epoxy resins either as a whole or as a part of a multi-coat system. Hybrid coatings based on acrylates, on the other hand, show good properties and offer promising results in the field of protection of steel and other metals. The siloxane-poly (methyl methacrylate) (PMMA) coatings presented the best features. In last years, there have been many studies which were focused on the development and improvement of siloxane-PMMA synthesis to obtain better corrosion protection. Most of the studies have been focused on the optimizing the molar ratio of precursors to obtain the improved properties of the coatings[1]. However, none of the studies has been devoted to the synthesis of coatings using different monomers with different functional groups. The goal of our work is to synthesize coatings with new functional groups in order to achieve improve corrosion protectiveness and hydrophobic characteristics in comparison to the already optimized reaction [1]. By modifying the reaction with the new monomers we expect to achieve improved properties of the coating which will be investigated by analysing their electrochemical properties and corrosion resistance, stability, durability and hydrophobicity. The current siloxane-PMMA coatings have a water contact angle of about 70° and with new monomers we will try to achieve higher contact angles, up to 120° or even more. This kind of coatings with hydrophobic or superhydrophobic properties would repel water and prevent corrosive species (Cl^-) to penetrate through the coating to the substrate.

To investigate the effect of various monomers on the properties of the coating we first used ethyl methacrylate as a monomer with additional -CH_2- group (R = Et, R^1 = Me). Siloxane-PMMA coating with methyl methacrylate was used for comparison with the new coating. In both cases the protective layers were applied on aluminum alloy substrate AA7075-T6. The coatings, which contained different acrylates, behaved similarly exhibiting comparative properties (contact angle, resistance value, and adhesion). In our future work, we aim to synthesis a sol with monomer containing longer linear alkyl chain expecting higher hydrophobicity of coating.



R: Me, *n*-alkyl, *n*-Fn-alkyl, *i*-alkyl, Ph
R1: Me, *n*-pentyl, *n*-dodecyl

Fig. 1. Schematic presentation of acrylate derivative

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Surface functionalization of barium hexaferrite nanoplates with promesogenic molecules

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Barium ferrite ($BaFe_{12}O_{19}$) is a hexagonal ferrite (BHF). It is distinguished with high magneto-crystalline anisotropy, due to which it crystalizes in the form of thin hexagonal plates having a magnetic easy axis perpendicular to the basal plates' plane. BHF nanoplates dispersed in nematic liquid crystal form fluid ferromagnetic phase[1]. It was reported that the colloidal stability of nematic liquid-crystalline suspensions containing inorganic nanoparticles can be improved by the surface functionalization with promesogenic ligands[2]. Promesogenic ligands contain mesogenic units, which also constitute the liquid-crystals molecules, and are responsible for the liquid crystals' properties. In addition, promesogenic ligands at the surface of nanoparticles can promote the alignment of the liquid crystal molecules.

Our aim was to functionalize the surface of the BHF nanoplates with promesogenic ligands that will allow for their dispersion in liquid crystalline matrix. We chose dendritic ligand with a phosphonic anchoring group and three mesogenic groups. The nanoplates were synthesized hydrothermally and stabilized in water at a pH of 3.5. Since the selected ligand is hydrophobic and soluble only in some nonpolar solvents, it was necessary to hydrophobize the nanoplates. Up to now, we studied two different procedures: 1) ligand exchange and 2) functionalization at a phase boundary. In the procedure 1) the as-synthesized nanoplates were primarily hydrophobized with ricinoleic acid that was subsequently exchanged with promesogenic ligands. The functionalized particles formed a stable suspension in toluene. In the procedure 2) we used bare nanoplates dispersed in water, while the promesogenic ligand was dissolved in toluene. Aqueous suspension of the nanoplates was subsequently added to the toluene solution. They were separated with a visible phase boundary: brownish aqueous part (due to brown nanoplates) at the bottom and transparent toluene solution at the top. The transition of nanoplates into the organic phase occurred immediately after the mixing of the two phases, which was observed visually: the top solution turned brown while the bottom solution faded. Functionalized nanoplates formed a stable suspension in toluene.

The functionalized BHF nanoplates aggregated in nematic liquid crystalline phase of 5CB. However, those prepared by procedure 1) redispersed when heated above the nematic-isotropic phase transition temperature.

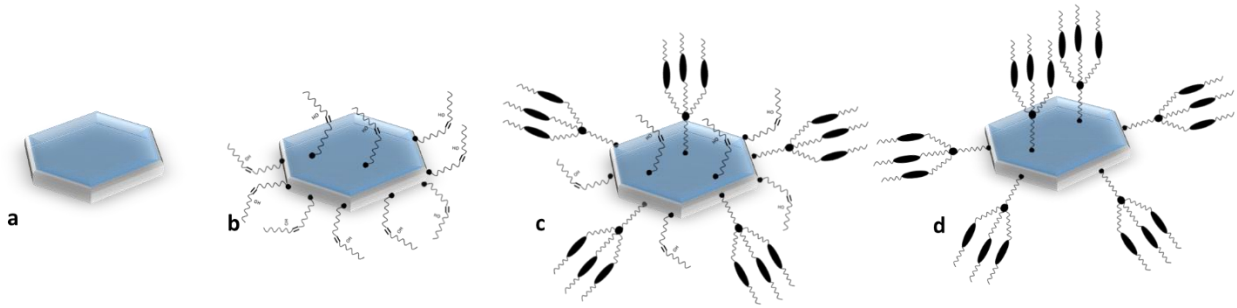

Figure 1: Schematic presentation of the nanoplate: a) bare, b) functionalized with ricinoleic acid c) after the ligand-exchange and d) after the functionalization at phase boundary.

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Lipid droplets are targets for reducing cancer resistance to stress

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During evolution, organisms have developed mechanisms to monitor and respond to changes in nutrient availability. Cells adapt to nutrient starvation by shifting their metabolism from reliance on glucose to dependence on mitochondrial fatty acid (FA) oxidation. Cells store FAs in the form of lipid droplets (LDs), newly recognized organelles, which are emerging as central hubs of lipid metabolism from yeast to men [1]. LDs are composed of a neutral lipid core containing triacylglycerols (TAG) and cholesterol esters surrounded by a monolayer of phospholipids and proteins. Cancer cells are often exposed to nutrient and oxygen deprivation due to their rapid proliferation and inadequate vasculature. The inability to synthesize their own FAs during stress forces cancer cells to scavenge extracellular lipids or to recycle intracellular lipids through autophagy [4]. Indeed, recent studies suggest that degradation of membranous organelles by autophagy provides FAs for LD biogenesis, whereas lipophagy, an LD-selective form of autophagy, may also participate in LD breakdown. We have shown that LDs protect breast cancer cells from starvation-induced cell death [2, 3], but the mechanisms involved are not known. The main aim of this study is to define the relationship between LDs and autophagy in breast cancer cells exposed to stress. We will modulate autophagy by genetic and chemical means and analyze the effects on LD turnover and cell survival in nutrient-deprived breast cancer cells. Lipidomic and proteomic analyses will be performed to determine changes in LD lipid composition and identify LD-associated proteins involved in stress response and activation of lipophagy. We will genetically inactivate LD biogenesis in luciferase-expressing breast cancer cells and use a mouse xenograft model in the presence or absence of autophagy inhibitors to determine whether LDs and autophagy are important for tumor growth *in vivo*. The results of our study will provide new opportunities for targeting the most resilient and aggressive types of breast cancer.

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P-glycoprotein: a combined *in silico* approach towards identification of safer chemicals

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P-glycoprotein (P-gp) is a transmembrane protein, playing significant roles in the process of drug discovery, development and toxicological assessment. P-gp affects absorption, distribution, and elimination of different compounds and it is mainly expressed in intestines, liver, kidneys, heart, colon, and placenta. The expression of P-gp in the blood-brain barrier (BBB) has been associated with the restricted access of many compounds to the central nervous system. P-gp is responsible for resistance of cells to xenobiotics, particularly the anticancer drugs, giving rise to the multidrug resistance (MDR) phenomenon by mediating the active transport of these drugs from the intracellular to the extracellular compartment. Increased expression of P-gp is also implicated in decreased availability of HIV drugs at certain intracellular sites. Moreover, studies showed that P-gp contributes to decrease toxicity by removing compounds from cells in mammals and preventing intracellular accumulation. Consequently, it is advisable in the drug discovery process to pay attention to the likelihood of a compound under development being transported by P-gp, since this contributes to whether a compound actually reaches its intended target or it is removed from the cell before exerting its action. Hence, *in silico* models for predicting the probability of interaction with P-gp in the early phase of drug discovery process are highly recommended.

The project aims to develop *in silico* models including P-gp characterization of substrate specificity and transport. A database of approximately 2,400 compounds, experimentally tested as P-gp substrates, inhibitors and non-active, will be used to develop a classification model that could provide rapid and cost-effective screening platforms for the identification of P-gp ligands. Theoretical models of P-gp transport mechanism intend to predict the binding interactions between the protein and small substrates and inhibitors. Since the murine and human P-gp shares around 87% sequence identity, for molecular docking calculations the X-ray crystal structure of murine P-gp and the primary sequence of human P-gp will be employed to build a human P-gp homology model. The outcome of the molecular modelling is going to be combined with the predictions resulting from QSAR models developed within the project. The *in vitro* studies performed by project partners are going be used and compared with the *in silico* results in order to generate a two way validation and subsequent optimization.

Plasma-assisted bottom-up approach for the synthesis of vertically aligned carbon nanostructures using polymer gels

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Vertically aligned carbon nanostructures have attracted research interest for a wide range of applications from electrochemical energy storage devices, catalysis, and electronic devices to sensing devices due to their unique orientation, morphology, electronic properties and large surface area and edge effects[1]. Plasma enhanced chemical vapor deposition is considered as a new promising method for the large-scale synthesis of vertically aligned carbon nanostructures. In contrast, this study explores an alternative route with a plasma-assisted bottom-up approach for the synthesis of vertically aligned carbon nanostructures. Several studies showed that phenol derived gels can produce carbon nanostructures by carbonization process[2,3]. So that, resorcinol-formaldehyde, phenol-formaldehyde and other polymer gels were used as a precursor for a carbon source in this study. A radiofrequency capacitively coupled plasma was used for the synthesis process, where a thin layer of polymer gel was cast on the substrate and placed in plasma. Argon and hydrogen gas species were used in the surface treatment and the carbon nanostructure supported growth at different discharge parameters. Various substrates were tested in order to investigate the effect of substrate on the orientation of carbon nanostructures. Moreover, the study explored also the influence of gas flow rate, the substrate temperature, and the growth time on the orientation and morphology of the carbon nanostructures.

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Influence of processing conditions on crystallinity and orientation of poly-L-lactic acid films prepared by tensile drawing

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Many studies confirmed that electric stimulation has a positive effect on treatment of bone fractures, which can be also achieved with piezoelectric polymers, even though they have smaller piezoelectric effect than ceramics [1]. Bone remodelling was already explained in 19th century with Wolff's law, which determines bone formation and resorption in response to stress, due to electrical potential, formed by piezoelectric nature of bone through body and muscle movement. Different piezoelectric materials are used for bone regeneration, which enables cell attachment and proliferation, usually in form of 3D porous structures, films and nanofibers, referred as scaffolds, depending on its purpose [2]. The idea is that piezoelectric polymer will induce regeneration process, so bone would gain its initial strength and function. In this study, piezoelectric, biocompatible and biodegradable polymer poly-L-lactic acid (PLLA) was used in form of films, for different potential applications as coatings for bone implants or directly as scaffolds for regeneration of bone or other tissues. Because of biodegradability of PLLA within three years, depending on its crystallinity, no later removal is needed [3]. Also *in vivo* studies of other authors showed promoted callus formation for drawn PLLA rods compared to undrawn polymer, with indirectly measured piezoelectricity [4].

In our study, a film of PLLA was prepared by uniaxial tensile drawing using a homemade stretching device. Since it has been shown that crystallinity and crystal orientation in polymer influence piezoelectric properties of mentioned polymer [5], different processing conditions of polymer film preparation were researched, to achieve higher crystallinity and orientation. Influence of strain, drawing temperature, draw rate and additional annealing on uniaxial stretched films for the purpose of achieving higher piezoelectricity were studied. Results showed that draw ratio and temperature have high impact on strain-induced crystallization and orientation on polymer films, which was confirmed with differential scanning calorimetry and scanning electron microscopy. X-ray diffraction and Fourier-transform infrared spectroscopy showed that as-prepared materials have disordered α' crystal form, however with additional annealing, polymer is transformed into more stable α form with increased crystallinity. Also optimal drawing temperature and rate for higher strain induced crystallization will be discussed.

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Capturing the Sun in a tungsten "box"

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Sun is the source of all energy in the Universe, even on Earth. Solar, wind energy, even fossil fuels and biofuels depend on sun. These processes are all indirect. However, what if we could make our star here on earth that would give us enormous amounts of energy?

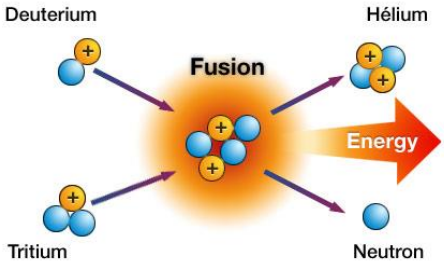

Figure 1: D-T fusion reaction

We can already replicate similar nuclear reaction happening on the Sun; fusion of light elements. In reaction between deuterium and tritium (D-T) large amounts of energy is released as by-product (Figure 1). However, at the moment in fusion reactors, we can control D-T fusion for several minutes. In order to fuse small nuclei, they must collide together with high energy at the rate of 100 million degrees. This hot plasma must be confined inside fusion reactors using strong magnetic field. One of the problems of designing a large fusion reactor that will be ignited for days/months is using the appropriate material that will withstand the harsh conditions. High thermal fluxes, thermal shocks and neutron irradiation are just a few of the conditions that plasma facing materials have to withstand after exposure to it for a long time.[1]

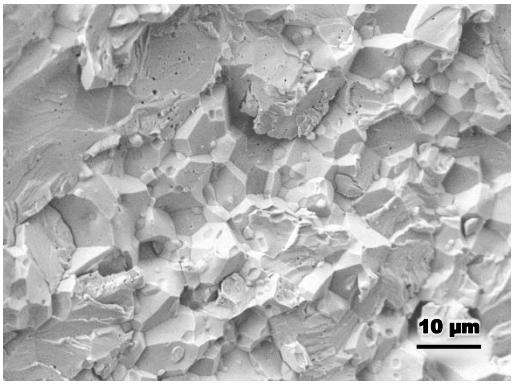

Figure 2: SEM image of W-WC composite sintered with field assisted sintering technique (FAST)

Tungsten is a primary candidate for this job, because of its favourable thermo-mechanical properties. Nevertheless, it has some disadvantages, which we are trying to overcome. Pure tungsten loses good mechanical properties at temperatures above 1000 °C, due to recrystallization accompanied by grain growth. The research at JSI confirmed that with the addition of small tungsten carbide particles into the metallic matrix, we could inhibit this undesirable processes and retain good mechanical properties even after exposing it to temperatures of 1600 °C for 24h. Our work is focused on optimizing the preparation of a W-W_2C composite: i) selection of the proper amount of the precursor for W2C particle reinforcement, ii) sintering techniques and parameters, iii) microstructure analysis (SEM, TEM, EBSD)(Figure 2) and finally iv) characterization of mechanical properties (strength, toughness) [2, 3]

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Effect of barium-hexaferrite nanoplatelets in low-frequency magnetic field on cancer cells

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Our studies were focused on a proof of concept of a novel cancer treatment, which is based on the transformation of low-frequency magnetic-field energy (1 Hz to 100 Hz) to mechanical energy. Such effect could be achieved through actuation of anisotropic magnetic nanoparticles, e.g., barium-hexaferrite nanoplatelets (BFNPs) internalized into cancer cells with an applied field. Barium hexaferrite is a hard magnetic hexagonal ferrite that grows in the form of platelets. The BFNPs display a high, uniaxial magneto crystalline anisotropy with an easy axis perpendicular to the nanoplatelet; a very rare property, which enables effective alignment of the platelet with the applied magnetic field. Exposure to a low-frequency alternating magnetic field causes the rotation of the nanoplatelets, which subsequently results in a mechanical torque that can be transferred to the surroundings (Figure 1). The BFNPs internalised into a cancer cell could therefore transfer the mechanical force to the cell organelles, causing damage to the cell.

The BFNPs, approximately 50 nm wide and 3 nm thick, were hydrothermally synthesized and subsequently coated with a thin silica layer, using a modified Stöber process. The silica-coated BFNPs were then grafted with dextran that was pre-reacted with (3-Glycidyloxy-propyl)trimethoxy-silane. Covalently bound dextran coating ensured the colloidal stability of BFNPs in physiological media by steric repulsive forces. Highly invasive, breast adenocarcinoma (MDA-MB-231) and cervical adenocarcinoma (HeLa) cancer cells were used for nanoplatelets cytotoxicity screening. Preliminary studies on biocompatibility and cytotoxicity of BFNPs were evaluated in *in vitro* studies using the Presto blue viability assay. Cells were incubated with different concentrations of BFNPs and treated with alternating magnetic field (2 Hz or 10 Hz) for a short period of time. There were no changes in cell viability in the absence of the field, proving the BFNPs are not toxic to the cells. On the other hand, cells treated with BFNPs and exposed to a magnetic field displayed a significant reduction in viability in comparison with control cells without BFNPs (Figures 2 and 3).

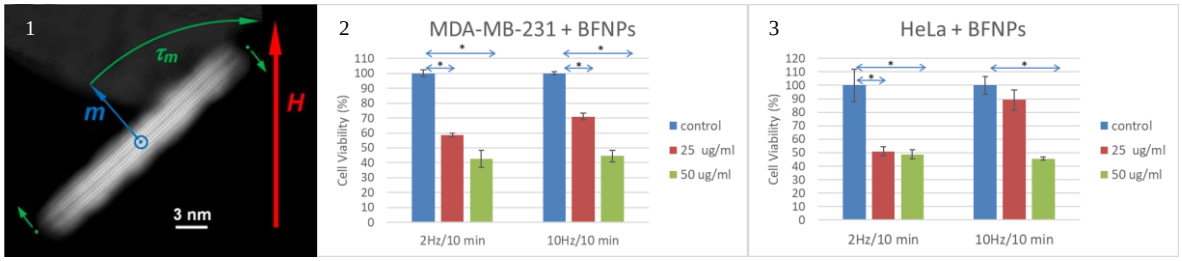

Figure 1: Atomic-resolution HAADF-STEM image of BFNP oriented edge-on with a schematic representation of the nanoplatelet's magnetization (***m***) and its rotation in a magnetic field (***H***) producing a torque τ_m; Figures 2 and 3: Viability of MDA-MB-231 and HeLa cells assayed by the Presto blue viability assay (*shows that the pair is statistically different: $p < 0,05$)

Acknowledgements:
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Lipid droplets – metabolic and signalling hubs involved in breast cancer survival during stress

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Lipid droplets (LDs) are dynamic organelles that store and supply lipids in all eukaryotic and some prokaryotic cells. Their unique structure, a core of neutral lipids, including triacylglycerols (TAGs) and cholesterol esters, surrounded by a phospholipid monolayer embedded with proteins, separates them from lipoproteins and requires specialized mechanisms for their formation, growth and breakdown [1]. LDs are important for the trafficking of exogenous and endogenous fatty acids (FAs) and are involved in regulating cellular lipid metabolism [2]. Secreted phospholipase A_2 ($sPLA_2$) enzymes release unsaturated FAs from plasma membranes of breast cancer (BC) cells and induce the formation of LDs, which enable cell survival during nutrient stress [3]. LD breakdown is crucial for protection of BC cells against starvation-induced cell death, but its molecular mechanism is not clear. Adipose triglyceride lipase (ATGL) is the rate limiting enzyme in LD degradation, which cleaves TAGs and mediates the transfer of FAs from LDs to mitochondria in mouse fibroblasts, but it may also control the synthesis of eicosanoids, lipid-derived signalling molecules involved in inflammation and cancer [2], [4]. The aim of our study was to examine the role of ATGL in supplying LD-derived FAs for cell survival during stress and for the synthesis of eicosanoids in BC cells. We found that ATGL depletion leads to reduced LD breakdown and cell survival during starvation, but, surprisingly, it was not necessary for $sPLA_2$-induced cell survival [5]. On the contrary, ATGL depletion reduces $sPLA_2$-induced prostaglandin E_2 synthesis, revealing a novel role for LDs and ATGL in the production of pro-tumorigenic eicosanoid signalling molecules in BC cells. In summary, LDs integrate metabolic and signaling pathways in cancer cells and are viable targets in the fight against aggressive breast cancer.

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Enhanced invasion capacity of glioblastoma cells after Kinin-B1 receptor activation and its involving in heterohybridism of mesenchymal stem/stromal cells

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Glioblastoma multiforme (GBM) represents the most lethal brain tumour, and these tumours have very limited treatment options. Mesenchymal stem cells (MSC) are considered as candidates for advanced cell therapies, due to their tropism towards GBM, possibly affecting their malignancy, thus also representing a potential therapeutic vector. Therefore, we aimed to compare the effects of bone-marrow-derived and adipose-tissue-derived MSC (BM-/AT-MSC) on heterogeneous populations of tumour cells. This cells' interplay was addressed by the *in-vitro* two-dimensional (monolayer) and three-dimensional (spheroid) co-culture models, using U87 and U373 GBM cell lines. U87 cell expressed high levels of kinin receptor 1 (B1R) and their migration/invasion was greatly enhanced by the B1R agonist des-Arg^9-bradykinin as well as blocked by B1R antagonist upon BM-MSC co-culturing in 3D co-cultures. This correlated to significantly higher cell-cell interactions (heterotypic fusion, vesicle transfer and cell cannibalism) observed in U87/BM-MSC coculture. Thoses cell-cell interaction between GBM and MSC were reduced after treatment with B1R antagonist (R715). We also demostrated the MSC makert acquisition phenotype by U87 cells after coculturing with BMMSC. Interesting that BM-MSC increase the cell survival rate and drug resistance of U87 and U373 GBM cells. Altogether, these data support the on-going exploration of kinin receptor B1R as target for adjuvant approach in GBM therapy. Secondly, the results emphasize the need for further careful exploration of the selectivity regarding the origin of MSC as potential candidates for cell therapies, particular in cancer, where they may adversely affect heterogeneous tumour formation.

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Optimization of zirconium based conversion coatings applied on aluminium alloy ENAB-AlSi7Mg0.3

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Currently there are numerous studies focusing to find comparative replacement process for chromium conversion coatings (CCCs) such as sol-gel process, conversion coating process based on rare-earths, transition metals such as molybdenum, vanadium, zirconium, titanium, trivalent chromium process (TCP), etc. Zirconium, titanium conversion coatings and TCP are already industrially commercialized but their corrosion performance is still behind that of CCCs. Zirconium conversion coatings are from 20 to 100 nm thick and consist of ZrO_2, ZrF_4 and $Zr(OH)_2$ formed from conversion coating bath based on hexafluoro zirconic acid, H_2ZrF_6, acid and different additives.

Our aim was to investigate the influence of H_2ZrF_6 acid concentration and treatment time on the corrosion performance of aluminium alloy (AA) ENAB-AlSi7Mg0.3. Samples were ground up to 4000-grit with SiC papers, ultrasonically cleaned with ethanol for 5 minutes and chemically cleaned in alkaline bath. Immediately afterwards, the samples were treated in H_2ZrF_6 conversion coating bath for different immersion times from 0.5 min to 3 min at room temperature. The H_2ZrF_6 concentration was: 100, 125, 150, 175, 200, 300, 500 ppm, pH was set at 4.8 and stirring rate was 450 rpm. The effect of bath temperature and pH was checked at optimal conversion bath concentration. The performance of conversion coatings was investigated by electrochemical measurements in 3.5% NaCl solution.

Zr-based conversion coatings act as cathodic inhibitors, shift the open circuit potential of AA towards negative potentials, increase its passive region for about 0.35 V and decrease corrosion current density. They represent a good basis for further development as chromate replacement.

Hybrid sol-gel coatings for corrosion protection of aluminium alloy 7075-T6

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Hybrid sol-gel coatings are amongst the most promising and environmentally friendly replacements for chromate conversion coatings (CCCs) for corrosion protection of aluminium alloys. They combine inorganic and organic components; the former offering good mechanical properties, and the organic components increasing the flexibility and ductility of coatings, with decreased treatment temperature. In the present work they were based on (3-glycidyloxypropyl) trimethoxysilane (GPTMS) and tetraethoxysilane (TEOS) and, by the dip coating technique, applied on aluminium alloy AA7075-T6. SiO_2 nanoparticles were added to the sol-gel solution to achieve barrier property of coating, while $Ce(NO_3)_3$ was added to obtain an active corrosion protection. The optimization of sol synthesis, opening of the epoxy rings and completion of hydrolysis and condensation reactions were confirmed by Attenuated Total Reflectance-Fourier Transform Infrared spectroscopy (ATR-FTIR) and Ultraviolet-visible spectroscopy (UV-vis-NIR). Moreover, a high degree of cross-linking between GPTMS and TEOS was achieved, in situ, during the synthesis and the effect of curing process on coating's properties was confirmed [1]. A double-layer system was developed and applied on AA7075-T6. The first layer of double system was doped with $Ce(NO_3)_3$ and the second was undoped. It was found out that cerium has a role in the self-healing if it is "locked" within the first layer of double-layer coating [2]. Coating characterization was carried out by the immersion test and electrochemical measurements, potentiodynamic (PD) and electrochemical impedance spectroscopy (EIS). The self-healing effect was confirmed by immersion of un-scribed and scribed coated AA7075-T6 in electrolyte NaCl by using the immersion test, EIS, X-ray photoelectron spectroscopy (XPS) and scanning electron spectroscopy equipped with energy dispersive spectroscopy (SEM/EDS).
One of the novelties of the present study was the increase in impedance at low frequency after 4 days of immersion for scribed coatings, which directly proves the self-healing (Fig.1).

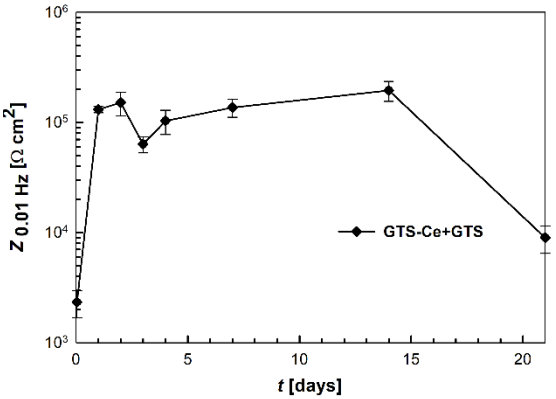

Figure 1: The impedance at 0.01 Hz, determined from Bode plots, of the magnitude of impedance vs. frequency recorded for a scribed GTS-Ce+GTS coating deposited on AA7075-T6 after various immersion times in 0.1 mol/L NaCl.

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Novel multicomponent Nd-Fe-B permanent magnets for energy conversion

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In the past few decades, Nd-Fe-B permanent magnets have become vital components of different devices and are used for efficient conversion of mechanical to electrical energy and vice versa. Wind turbines, for example, work on the principle of electromagnetic induction and large permanent magnets are used for cost-efficient, pollution-free generation of electricity. Similarly, magnets are needed in electric motors that are found in home appliances (e.g. air conditioners, refrigerators and washing machines), automobiles (fuel pumps, windscreen wipers, electric steering) and (hybrid) electric vehicles. They are also used in computers, cell phones, microphones and speakers.

An important property of a magnet is its intrinsic coercivity (H_{ci}), a measure of the magnet's ability to withstand the external demagnetizing fields. Coercivity depends on the magnet's microstructure, with nanostructured materials having the highest H_{ci} values. Even higher H_{ci} can be achieved with the addition of heavy rare earth (HRE = dysprosium or terbium) elements to the Nd-Fe-B alloy. However, HREs are expensive and critical raw materials, therefore their use should be minimized. In addition, Dy and Tb reduce the magnetic flux density and consequently the power output of the magnet-containing device.

Intrinsic coercivity deteriorates with the increase in the temperature. Magnets such as the ones used in (hybrid) electric vehicles operate at high temperatures (> 100 °C) and under large reverse magnetic fields that tend to demagnetize the exposed regions of the magnet. Those regions therefore need to contain a high-coercivity material. Large concentrations of Dy or Tb (up to 10 wt%), homogeneously distributed throughout the magnet body, are used in commercially available sintered magnets. To minimize the demand for HRE elements, we developed a novel approach and prepared a nanostructured multicomponent magnet containing a HRE-free and a Dy-containing region [1]. Two nanostructured Nd-Fe-B powders with different compositions and magnetic properties were consolidated into a dense bulk magnet with a rapid hot pressing technique called "Spark Plasma Sintering" (SPS). In order to retain the respective H_{ci} values of the original materials, low temperatures were used and the grain growth during the SPS process was therefore prevented. The results of the magnetic characterization showed that distinct regions with different magnetic properties exist in the multicomponent sample.

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Metal oxide anchored graphene-gold nanoparticle hybrid electrodes for energy applications

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ABSTRACT

Graphene, the hexagonal monolayer of carbon (C), has been playing the leading role in the research of flat 2D materials due to its unique physical and electronic properties. It has been proved that graphene can serve as a perfect 2D support for anchoring metal or metal oxide nanoparticles[1]. Anchoring metal oxides on graphene/gold hybrid electrode would enhance the electrochemical properties of material depending on its structure, size and crystallinity. Chemically converted graphene sheets can be obtained from graphite and can be stabilised in aqueous colloids through electrostatic stabilization[2]. Graphene–gold nanoparticles (AuNPs) hybrid can be fabricated by the reduction of $HAuCl_4$ using hydrazine followed by sodium citrate[3]. Nano-sized oxide particles anchored on the surface of Graphene/AuNPs hybrid or wrapped within the hybrid could be synthesised using the synergistic effect acting between graphene and different metal oxides. When it is used for electrode materials, the graphene- AuNPs/ metal oxide composites, with which individual structural variables like anchored or wrapped, should have a substantial improvement in their electrochemical properties such as high specific capacity, high rate capability, high energy density and excellent cycling stability as compared to their constituents. Combined advantages of both graphene/AuNPs hybrid and metal oxides results in improving the electrochemical energy storage, lowering the current electrode problems of the individual components of graphene or metal oxides as active materials.

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Drugi programi (Other programs)

Hexanucleotide $(C_4G_2)_n$ RNA repeats sequester RNA binding proteins

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The most common genetic cause of two incurable, progressive neurodegenerative diseases - amyotrophic lateral sclerosis (ALS) and frontotemporal dementia (FTD) is *C9ORF72* gene mutation. This mutation causes up to 40% of hereditary and 5-10% sporadic cases of ALS and 25% of hereditary FTD cases. ALS and FTD share clinical, neuropathological and genetic characteristics.

C9ORF72 gene is a non-characterized human gene; the mutation occurs in a non-coding part of the gene, resulting in an increased number of polymorphic hexanucleotide repeats of GGGGCC. The number of repeats varies among individuals; in healthy individuals there are almost never more than 23 repeats present, in the case of patients, the number of repeats is equal to several hundred or several thousand.

Three different mechanisms of action are proposed for the *C9ORF72* mutation: haploinsuficiency of C9ORF72 as a result of reduced expression of the gene with the present mutation; the toxicity of RNA molecules transcribed from hexanucleotide repeats and the toxicity of proteins with dipeptide repeats (DPRs), which are product of a non-classical translation of hexanucleotide repeats. These mechanisms are not mutually exclusive.

Our research is focused on the RNA toxicity of hexanucleotide repeats. Extended hexanucleotide repeats in the intron of the *C9ORF72* gene are transcribed into RNA in the sense (G_4C_2) and antisense (C_4G_2) form. The resulting RNA molecules can form different secondary structures - loops, lashes, DNA-RNA heteroduplexes, RNA-duplexes, G-quadruplexes, I-motives. Stable secondary RNA structures allow the formation of RNA foci in the nuclei of neurons in spinal cord and brain of C9 ALS / FTD patients.

Formation of RNA foci was also noticed in other diseases with extended repeats of a particular sequence, such as myotonic dystrophy, where RNA foci are sequestering different RNA binding proteins and thus withdraw them from normal cellular functions. A similar mechanism is predicted for the *C9ORF72* mutation in ALS / FTD. We will present our latest findings about longer, biologically relevant repeats of the antisense C_4G_2, their binding proteins and relevance of this interaction for disease processes.

The influence of mercapto, benzene and methyl groups of imidazoles on the corrosion inhibition of aluminium based metals

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Corrosion is interesting phenomenon that is considered to be an unwanted spontaneous electrochemical reaction that can lead to the structural degradation of a material. Cost related to corrosion are estimated to be around 3.5 % of the G.D.P. of industrialised societies [1]. In the US Air-Force these costs amount to over $1 bn per year. The ultimate goal of a corrosion engineer is to predict and control the rate of corrosion. To do so, it requires a thorough understanding of the thermodynamic and kinetic fundamentals. Corrosion inhibitors, added to an environment to decrease the rate of corrosion of metals exposed to that environment, have been known for decades and they are considered as one of the most important methods of corrosion protection. The 2024 aluminum alloy, with copper as the primary alloying element, is widely used in the aerospace industry due to its high strength-to-weight ratio. The alloy is composed of intermetallic particles, which can form galvanic couples, and further in contact with moisture and aggressive electrolyte promote localized corrosion. Therefore, aluminium alloys have to be protected to sustain corrosion attack. Although the chromate coatings offer good corrosion protection, they are considered to be environmentally unfriendly and should be replaced.

The family of imidazole organic compounds has been recognized as effective green inhibitors for copper metal. It is well known for inhibitors that presence of hetero atoms (N, O, or S) with lone electron pairs and/or aromatic rings with delocalized π electrons enables them to adsorb to the metal surface and form protective complex layers [2]. Pronounced differences were observed at concentrations ≥1 mM. The mercapto and benzene group have shown to have a beneficial effect on corrosion inhibition, whereas the effect of methyl group is different accelerating the corrosion, especially at higher concentrations. Benz-, and mercapto- derivatives, that are superior to plain imidazoles, have strong effects on both the anodic and cathodic reactions shifting E_{corr} to positive values, and they are considered to be mixed inhibitors for copper.

The aim of present work is to first upgrade the previous work [3], and investigate the kinetics of corrosion of aluminum metal coated with imidazole derivatives. As the second step, a novel approach will be carried out by exploring the effect of using the inhibitor mixtures (the one which is good for copper, and the one for aluminum) on corrosion rate of the alloy. The possible synergistic effect of inhibitors, as well as the mechanism of corrosion inhibition will be investigated by means of electrochemical polarization methods, i.e. linear polarization resistance and potentiodynamic curves.

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Density functional theory study of adsorption of azoles on $Cu_2O(111)$ model of oxidized copper surfaces

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This work investigates the interaction between imidazole, triazole, and tetrazole—used as archetypal models of azole corrosion inhibitors—and oxidized copper surfaces, where Cu_2O is used as a model of oxidized copper. Azoles (five-membered heterocyclic organic molecules consisting of one or more nitrogen atoms) and their derivatives are known for their ability to inhibit the corrosion of copper [1]. Because it is known that molecular adsorption represents an important step in achieving the inhibition of corrosion, several density functional theory (DFT) studies explained the bonding of azoles to reduced copper surfaces [2–4]. However, oxide-free copper surfaces are more relevant at acidic pH, but under other conditions copper surfaces are often oxidized. Due to that, we adressed the adsorption characteristics of three simple azole molecules on oxidized copper surfaces, where we considered bonding on coordinatively-unsaturated (CUS) Cu sites of $Cu_2O(111)$ and on coordinatively-saturated (CSA) Cu sites of $Cu_2O(111)$-w/o-CUS surface. It was found that all three azoles bind weakly to CSA sites ($E_{ads} = -0.5$ eV), whereas they adsorb about three times stronger to CUS sites. We constructed two-dimensional phase diagrams as a function of chemical potentials of oxygen and azole molecules. Results imply that bonding to CUS sites is so strong that it compensates the thermodynamic deficiency of stoichiometric $Cu_2O(111)$ thus making it more stable than non-stoichiometric $Cu_2O(111)$-w/o-CSA. From current results it can be suggested that the corrosion inhibition capability of azoles steams from their ability to passivate the reactive surface sites.

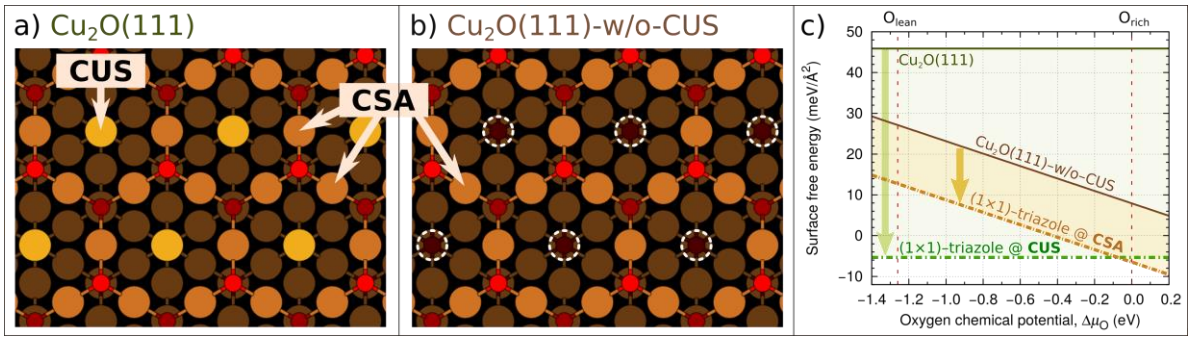

Figure 1: Structures of a) $Cu_2O(111)$ and b) $Cu_2O(111)$-w/o-CUS surfaces with indicated coordinatively unsaturated (CUS) Cu and saturated (CUS) Cu sites. c) Surface free energy of clean surfaces as a function of oxygen chemical potential and its stabilization due to molecular adsorption at CSA and CUS sites.

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Speciation of platinum-based chemotherapeutics in serum of cancer patients by conjoint liquid chromatography on monolithic columns

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Cancer is one of the leading causes of morbidity and mortality worldwide. For its treatment, Pt-based chemotherapeutics are commonly used in medicine. Among them, the most important are cisplatin, carboplatin and oxaliplatin. To better understand the pharmacokinetics of Pt-chemotherapeutics in cancer patients receiving chemotherapy and to reduce side effects of chemotherapeutics, it is necessary to understand their mechanisms of action and interactions with serum proteins. This information can be obtained by the application of the chemical speciation analysis.

In the investigations of the behaviour of platinum (Pt)-based chemotherapeutics, it is necessary to separate the intact drug and its individual species in serum samples. In speciation analysis of biomolecules, monolithic chromatography using convective interaction media (CIM) disks or columns hyphenated to ultraviolet (UV) and inductively coupled plasma mass spectrometry (ICP-MS) detection represents a powerful analytical tool.[1-3] CIM monolithic disks can be placed together in one housing forming so-called conjoint liquid chromatography (CLC) monolithic column. By assembling CIM Protein G and CIM diethylamine (DEAE) monolithic disks in a single housing, it is possible to accomplish two-dimensional separation by affinity and ion-exchange modes in a single chromatographic run.[4,5]

The CLC set-up may be constructed from CIM 0.34 mL shallow monolithic disks, forming low pressure CLC column (maximum 50 bar), or high pressure CLC column (maximum 150 bar) is constructed from 0.1 mL CIMac analytical high performance short bed monolithic disks. To achieve the best selectivity and robustness of the chromatographic separations, there is a need to test and compare the performances of low and high pressure CLC columns. In the present work, the potential of the low pressure and high pressure CLC columns bearing Protein G and weak anion-exchange CIM DEAE disks was evaluated in speciation of cisplatin, carboplatin and oxaliplatin in spiked serum proteins and spiked human serum. The robustness, repeatability and reproducibility of the analytical procedure on CLC columns were compared. The separated serum proteins were detected on-line by UV, while the elution Pt species by ICP-MS. For accurate quantification of the separated Pt species (unbound portion of the Pt-based chemotherapeutic from species associated to transferrin (Tf), human serum albumin (HSA) and Immunoglobulin G (IgG)), post column isotope dilution (ID)-ICP-MS was used. Finally, the analytical methodology was applied in speciation of Pt in serum of cancer patients.

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Electrostatic stabilization and geometric effects lead to attractive interactions between oxygen adatoms on aluminium surfaces

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When electronegative atoms adsorb on an electropositive metal surface, charge transfer occurs and the adatoms become negatively charged. Due to this charge accumulation, repulsive lateral interactions are expected between them, and according to the classical method of images they can be treated as dipole-dipole interactions that scale as $\Theta^{3/2}$, where Θ is the surface coverage of adatoms. This dependence is typical for chemisorbed atomic oxygen on transition metal surfaces and it is depicted in Figure 1a for atomic oxygen on Cu(111). However, in the case of O on Al(111) and Al(100) surfaces the opposite occurs and the magnitude of binding energy increases with increasing coverage (see Figure 1b). Analysis of the electronic structure with DFT calculations reveals that the attractive interactions are a consequence of a simple electrostatic stabilization. Namely, at full monolayer coverage the O adatoms are located close to the surface and together with positively charged surface Al atoms form an electrostatically stable interlaced layer of anions and cations. This is evident from Figure 1c which shows the charge density difference for O on Al(111) (note the alteration of positive (blue) and negative (red) regions). We conclude that the attractive interactions between negatively charged O adatoms at high-coverage stem from an interplay between Coulombic interactions and geometric effects (height of the adatoms), i.e. there exists a critical adatom height below which the lateral interactions are attractive and above which they are repulsive. We propose that this picture is generally applicable for electronegative adatoms on metal surfaces provided that (i) the adsorption bonding is sufficiently ionic and (ii) the adatoms are sufficiently small to come close enough to the surface.

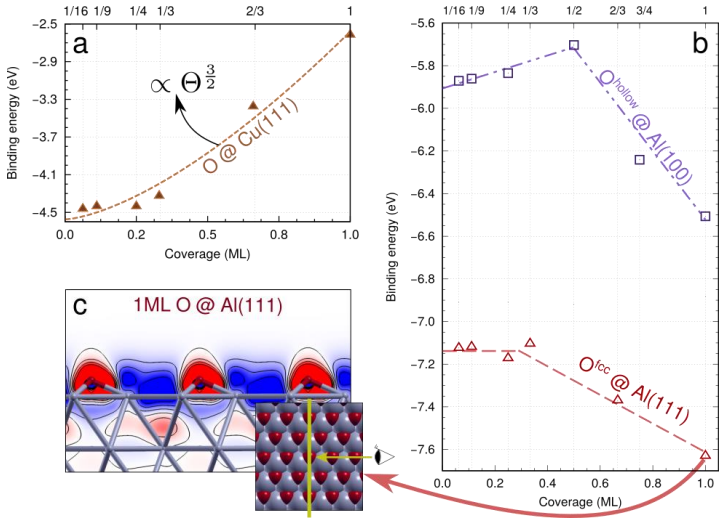

Figure 1: Binding energy of oxygen on (a) Cu(111) and (b) Al(111) and Al(100) with respect to coverage (Θ). (c) Charge density difference of 1 ML O @ Al(111); blue (red) color corresponds to electron charge deficit (excess) regions.

Regulation of effector function of cytotoxic T cells by cystatin F

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Cytotoxic lymphocytes include cytotoxic T lymphocytes (CTLs) and natural killer (NK) cells and represent the most important players in the immune response against tumour cells and infected cells due to their ability to directly kill target cells. Target cell death can be achieved by different pathways, the important one is the perforin/granzyme pathway. Here activation of cytotoxic lymphocytes triggers exocytosis of their cytoplasmic granules, named lytic granules, that contain perforin, granzymes and several other peptidases. Perforin is a pore-forming protein and mediates the penetration of granzymes into the target cells, where granzymes trigger an apoptotic cascade leading to cell death. Both, perforin and granzymes, are synthesised in an inactive pro-form and need to be activated by other peptidases. Granzymes are activated by cathepsins C and H, while perforin can be processed by cathepsin L. Activity of cathepsins is regulated by their endogenous protein inhibitors, the cystatins. In our recent work, we demonstrated an important role for cystatin F in regulation of cytotoxicity of NK cells. Since the molecular machinery involved in the cytotoxicity of NK cells and CTLs is the same, we hypothesized, that cystatin F could also be an important regulator of CTLs' effector function. Thus, we first established a model system using TALL-104 cell line that shares many characteristic features with human CTLs. In addition, we treated TALL-104 cells with low concentration of calcium ionophore ionomycin, mimicking unresponsive CTLs after prolonged stimulation with cancer antigens. In our model the cytotoxicity of TALL-104 was reduced, as measured by calcein-AM method, while the viability was unchanged. The protocol did not activate the cells, however, after appropriate stimulation, the cells released their granule content, as assessed by flow cytometry and LAMP1 labelling and by measuring granzymes B and A levels in cell media. Using western blotting we found increased levels of the inhibitor cystatin F in treated TALL-104 cells. Furthermore, proximity ligation assay and confocal microscopy revealed that cystatin F is co-localized with cathepsin C and granzyme B. Therefore, cystatin F is an important regulator that can impair CTL cytotoxicity.

Circulation model of wide-open bays

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Our research field is physical oceanography, which is the study of fluid dynamics in the ocean and coastal seas. The goal of our research is the simulation of water circulation in wide-open bays. A wide-open bay contains one 'long' side which is an open boundary line (OBL), with dimensions comparable to those of the coastline around the bay. This means that the exchange of water with larger water bodies could have a complex structure along the OBL and suppositions about the (fluxes of) quantities (temperature, salinity, currents, concentrations of pollutants) through it could be erroneous. We decided to simulate the circulation in such bays with the use of the Nucleus for European Modelling of the Ocean (NEMO) model with the concept of one-way nesting. The NEMO model numerically solves the equations of geophysical fluid dynamics that is the Navier-Stokes equation for a turbulent flow on a rotating Earth, along with a nonlinear equation of state, and the equation of continuity. The model relies on the following approximations: Spherical approximation for the Earth, thin-shell approximation, the Boussinesq hypothesis, hydrostatic hypothesis and the incompressibility hypothesis. With the method of one-way nesting fluxes of salt, heat and momentum through the OBL are passed from the coarser model, developed by the Slovenian Environment Agency (ARSO), to the finer model of wide-open bays. This means that the interpolation of quantities calculated by the coarser model is applied to a finer spatial grid of the smaller model domain. The model will be initialized with the field data of temperature, salinity and currents at the beginning of 24 h measurement campaigns and it will also be validated with the field data of currents at the end of these campaigns over the Bay of Koper.

The Gulf of Trieste, the Bay of Piran and the Bay of Koper as wide-open basins.

Investigation of arsenic in contaminated soils in the Mežica valley

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The Mežica valley has been exposed to more than three hundred years of active lead mining and smelting. Soils in the valley, including about 7000 ha of agricultural land, are polluted especially with Pb and Zn, but also with Cd and As. In 1990 the lead ore mining and smelting production stopped, to be replaced with recycling of old car batteries. At present there are two main sources of pollution: the lead smelter in Žerjav and landfill at Glančnik, where scoria and plastic parts of batteries are deposited [1]. The aim of this study was to investigate how arsenic is bound to soil components to assess the potential leachability and bioavailability, both important factors in evaluating the pollution risks. Nine soil samples (five from populated land in the valley and two from the ridge above Death valley, close to former smelting plant) were investigated using the BCR extraction scheme [2]. The BCR extraction scheme comprises three steps and targets the extractability of elements from specific soil component: *i*) exchangeable elements and elements bound to carbonate are extracted with 0.1 M CH_3COOH, *ii*) elements bound to iron and manganese oxides (reducible fraction, extractable with 0.1 M $HN_2OH{\cdot}HCl$ in HNO_3 at pH 2), and *iii*) elements bound to organic matter and sulphides (extractable with 30 % H_2O_2 and 1M CH_3COONH_4). The total arsenic concentration in sample extracts was determined using flow injection - hydride generation - atomic fluorescence spectrometry [3]. Our results show that arsenic pollution in and around the Mežica valley varies considerably, from unpolluted (< 10 μg g^{-1}) in some garden soils to heavily polluted (> 200 μg g^{-1}) in the top soil on the ridge above Death valley. The extractable arsenic (10-30 %) was found in an exchangeable/bound to carbonate fraction and in a fraction bound to iron and manganese oxides while most of arsenic is tightly bound to organic matter and sulphides (55 - 70 % of the extractable fraction). The most environmentally mobile is the exchangeable fraction, which also presents the highest potential danger to the environment. We plan to further investigate this fraction and subject it to determination of inorganic arsenic forms (arsenite and arsenate), next to studying the extractability and environmental mobility of lead, zinc and cadmium in these soils and potential expansion of this study to water and sediments from the Mežica valley.

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