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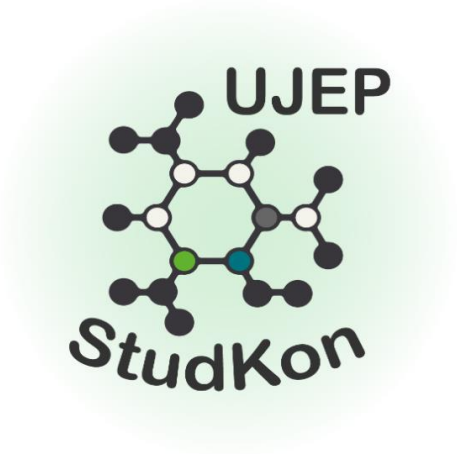

KNIHA ABSTRAKTŮ

4. Konference studentů přírodovědných a technických oborů UJEP

StudKon 2021

28. 6. 2021

Centrum přírodovědných a technických oborů

Univerzita J. E. Purkyně, Ústí nad Labem

http://www.studkon.ujep.cz

PROGRAM KONFERENCE

PONDĚLÍ 28. 6. 2021	
Registrace	**8:00 – 9:00**
Dopolední program	**9:00 – 13:20**
9:00 – 9:10	Zahájení a přivítání účastníků
9:10 – 10:30	Přednáškový blok 1
10:30 – 11:00	Coffee break
11:00 – 12:20	Přednáškový blok 2
12:20 – 13:20	Polední přestávka – oběd, instalace posterů
Odpolední program	**13:20 – 19:00**
13:20 – 13:50	Krátké představení posterů
13:50 – 15:10	Přednáškový blok 3
15:10 – 15:40	Coffee break
15:40 – 16:00	Diskuze nad výsledky dotazníku – Jiří Orava
16:00 – 17:00	Vystoupení hosta – Tomáš Wágner
17:00 – 18:30	Posterová sekce
18:30 – 19:00	Technická přestávka
Večerní program	**19:00 – 22:00**
19:00 – 19:30	Vyhlášení výsledků soutěže o nejlepší poster a přednášku – Cena M. Broula
19:30 – 22:00	Večeře / raut, volný program

PŘEDNÁŠKOVÁ SEKCE

PŘEDNÁŠKOVÝ BLOK 1 (9:10 – 10:30)

9:10 **Tomáš Lank:** Properties of sodium polyacrylate in the environment and its reuse as superabsorbent for water in accordance with circular economy

9:30 **Aloui Norchene:** Growth of zinc oxide nanorods on PDMS/ITO films for piezoelectric transparent flexible nanogenerators as a self-powered sensor for transportation monitoring

9:50 **Kristína Fiantoková:** Chemical recycling of Li-Ion batteries

10:10 **Jan Hubáček:** Dehalogenation during pyrolysis of plastics: The potential of stepwise pyrolysis in combination with metal sorbents

PŘEDNÁŠKOVÝ BLOK 2 (11:00 – 12:20)

11:00 **Viktorie Neubertová:** Surface grafting of Mxene flakes for magnetic resonance imaging

11:20 **Petr Panuška:** A microfluidic chip for cultivation of fish embryos and toxicity testing fabricated by 3D printing technology

11:40 **David Poustka:** Microfluidics for exosome isolation

12:00 **Eliška Rezlerová:** Methane, Ethane and Propane Adsorption and Diffusion in Dual-Porosity Kerogens from Molecular Simulations

PŘEDNÁŠKOVÝ BLOK 3 (13:50 – 15:10)

13:50 **Hana Burdová:** The impact of diesel pollution on Miscanthus x giganteus biomass - two years pot experiment

14:10 **Jakub Perner:** Study of fluidized bed reactors and their use

14:30 **Simona Lupínková:** Iron oxide nanoparticles immobilized on activated polymer surface

14:50 **David Kramoliš:** Preferential acceleration of heavy-ions in solar flares

POSTEROVÁ SEKCE

17:00 – 18:30

Petr Aubrecht	Stop-flow microfluidic system for the immuno-capture of CTC
Jan Dočkal	Molecular force field development for aqueous alkali halide electrolytes
Tereza Dušková	Metal complexes with polyfluorinated NHCs - synthesis and biological effects
Michal Hošek	Source of heavy metals in agricultural soils – man, or nature?
Adéla Jagerová	Surface modification by high-energy heavy-ion irradiation in various crystalline ZnO facets
Pavel Kaule	Deposition of thin layers of covalently bound heteroboranes on PES textiles
Martin Kozakovič	The effect of collision parameters and particle diameter on the dynamics of the mixing process by using discrete element method
Diana Nebeská	Nutrients deficiency affects Miscanthus x giganteus physiology and essential metals uptake more intensively than soil contamination
Zuzana Nejedlá	Uptake, biodistribution and elimination of carbosilane dendrimer in vivo
Robert Ato Newton	Potential of biochar application in the phytoremediation process and biomass production of Miscanthus x giganteus
Dominik Pilnaj	Sensorics and high resolution mass spectrometry for environmental analyses
Jiří Smejkal	Open-source technologies in biotechnological laboratories
Jan Štěpka	Antimicrobial effects of nanoparticles on complex microbial communities
Martin Šulc	Gypsum technology of separation Li_2CO_3 from Zinnwaldite mineral
Jakub Tolasz	Interaction of pollutants on nanoceria
Zuzana Žmudová	Biodistribution and cytotoxicity of phosphonium carbosilane dendrimer

Přednáškový blok 1
(9:10 – 10:30)

Properties of sodium polyacrylate in the environment and its reuse as superabsorbent for water in accordance with circular economy

*Tomáš Lank[a]

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The aim of this thesis is to offer alternative applications of wasted consumer goods with containing absorbing material based on sodium polyacrylate. Other known names are waterlock, superabsorbent or hydrogel. In all the world, sodium polyacrylate $(C_3H_3NaO_2)_n$ is commonly used as a major compound in disposable diapers. The sodium polyacrylate is derived from petroleum such as other plastics. [1] That is very easy to use and very comfortable for people to use only once and to throw them into a dustbin, but this molecule can be REused more times. I focused my topic on alternative reuse of sodium polyacrylate in the environment, e.g. absorptive material in hydroponic fields for planting vegetation in dry areas. Maybe it could help us to reuse this material in many cycles which is in harmony with circular economy in sources and wastes. So, it is better not only to dispose it after first use which is wasting of sources, but to reuse all advantages of this material.

The mechanism how to get secondary extracted non-infectious material from dirty disposable diapers is in wastewater treatment plant. Hydrogel is non compact lumpy material. In contact with water is the first step water absorbing. If there is over water capacity the hydrogel is hydrolytically separated for small parts. It needs more water than is full absorbing hydrogel capacity. These parts of hydrogel with wastewater are accessible for microorganisms in cleaning process. These microorganisms mineralize and clean the gel. Output of this process is sewage sludge with hydrogel and fertilizers. Next process is physically centrifugation which decrease content of water for transportation. Clean secondary extracted hydrogel is economically interesting material.

Figure 1 Circular model of wasted diapers recyclation

Research highlights

The sodium polyacrylate is non-toxic water absorbent that can absorb 300 times more weight of water than its own weight. It could be an alternative source for planting vegetation instead of potassium polyacrylate. Used hydrogel is perfect pure non-toxic material for pyrolysis. This is a basic idea of circular economy.

References

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Graphic abstract is compiled with listed internet sources:
Pyrolysis.In:lbgmoravia.cz[online],19.3.2021 10:30:02. Available:https://www.lbgmoravia.cz/technologie/zpracovani-odpadu/depolymerizace-plastu-p53/. Hydroponics.In:wikipedia.org[online],19.3.2021 10:32:02. Available: https://cs.wikipedia.org/wiki/Hydroponie, Hydroponics mechanism.In:pestik.cz[online],19.3.2021 10:47:02. Available: https://www.pestik.cz/module/csblog/post/72-14-hydroponie-pro-zacatecniky-.html#gref, Circular economy.In:zajimej.cz[online],19.3.2021 10:48:02. Available:https://zajimej.se/pracovni-pozice-budoucnosti-cirkularni-ekonomika-prinese-cesku-az-150-tisic-novych-mist/, Diaper.In:indiamart.com[online],19.3.2021 10:49:02. Available: https://www.indiamart.com/proddetail/baby-diapers-18460912712.html, Pyrolysis oil.In:indiamart.com[online],19.3.2021 11:02:02. Available: https://www.indiamart.com/proddetail/pyrolysis-oil-5961921155.html, Sodium polyacrylate.In:pestik.cz[online],19.3.2021 11:14:02. Available: https://www.alibaba.com/product-detail/Competitive-Price-Sodium-Polyacrylate-Degradable-Raw_1600057436508.html, hydroponic waste. In.gaiaca.com[online],19.3.2021 11:55. Available https://www.gaiaca.com/dispose-hydroponic-nutrients/.

Growth of zinc oxide nanorods on PDMS/ITO films for piezoelectric transparent flexible nanogenerators as a self-powered sensor for transportation monitoring

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Harvesting the energy from our living environment has been a crucial issue for sustainable development and has attracted long-standing interest since the beginning of this century.[1] Recently,a piezoelectric nanogenerator (NG)- has been developed to convert mechanical energy into electrical energy through the coupled piezoelectric and semiconducting properties of ZnO nanostructures. ZnO is an excellent material for the application in sensors because it improves sensitivity and it is one of the piezoelectric materials that can transform mechanical stress / strain into electrical voltage due to the relative displacement of cations and anions in the crystal.[2]The objective of this study is to develop a piezoelectric thin film characterized by high piezoelectricity and favorable mechanical properties. [3]This work endeavors to report on the development of a high aspect ratio ZnO nanorods, ~4–5μm long and ~300–500 nm in diameter – aspect ratio of up to 17:1 used for piezoelectric NGs.The seed layer solution of ZnO nanocrystals, is formed by dissolving zinc acetate dehydrate in ethanol as a precursor.An equimolar solution of zinc nitrate hexahydrate and hexamethylenetetramine (HMT) was dissolved in deionized water.The addition of polyethylenimine (PEI) into the growth solution examined in this work in terms of the aspect ratio of formed ZnO nanorods [4].Based on the final device architecture and its characteristic, we aim to demonstrate its application as a self-powered sensor for monitoring vehicles speed and detecting their weight.This study offers a novel approach ZnO-CNT nanotubes (NTs),one of their potential applications is the pressure/stress sensors based on their vibration sensitivity to external pressure.

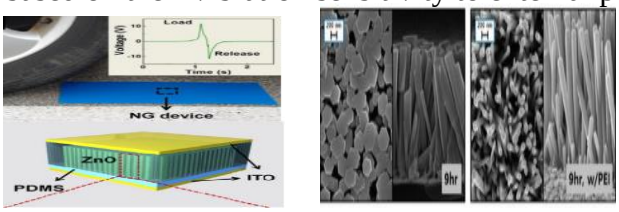

Figure 1 Left part: structure and working principle of a transparent flexible nanogenerator (TFNG). Right part: SEM micrographs of the as-grown ZnO NW arrays composing a self-powered sensor for transportation monitoring. [1]

Reaserch Highlights

1) Study the variation in the hydrophobicity of the PDMS was characterized by measuring the contact angle of a liquid droplet against the surface of the PDMS.
2) Demonstrate the enhancement of output power from a ZnO nanorod (NR) based piezoelectric nanogenerator
3) Study the effect of polyethyleneimine (PEI) on the structure and micro-morphology of ZnO nanorod array film
4) Optimization of processing parameters on the controlled growth of ZnO nanorod array

References

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Chemical recycling of Li-Ion batteries

Pavel Janoš[a], Jiří Štojdl[a], *Kristína Fiantoková[a], in cooperation with the IBG Czech Ltd.

[a]Faculty of Environment, J. E. Purkyně University in Ústí nad Labem, Czech Republic

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The project focuses on the research and development of processes in the field of energy and material recycling of the Li-Ion batteries. In order to implement new concepts of disposal of the industrial usage of the batteries according to the principles of circular economy, means to develop a complex system, which uses residual battery voltage (this is called „second life“ system). Batteries, which can no longer be used for the „second life“ system, become a secondary source of materials – this is the subject of the material recycling, including chemical and other processes to obtain valuable elements from the used batteries.

The „second life“ system includes the collection and sorting of the batteries and their usage in a special high-capacity storage. The focus is mainly on the Li-Ion batteries, used in electric vehicles and handling equipment. However, it is possible, to extent the project also on other types of batteries, as long as they have a relevant market share/need.

Nowadays hydrometalurgical and pyrometalurgical treatments are mostly used when it comes to the recycling of the batteries. By these technics there is a high consumption of energy, as the temperatures starts at least by 500 – 600°C and can further rise. In a purpose of a new designed concept for the entire recycling process, we are going to use a mixture, which consists of sulfuric acid and hydrogen peroxid, which is called piranha solution. By applying of this mixture in the chemical treatment part, there is no need to heat up the formed black mass (it is a composition of platic, metal and electrolyte), as the mixture itself is very exotermic.

In the chemical part of recycling also ultrasound will be applied as a further aspect of the selection process, which helps to increase the acceleration and the effect of the piranha solution on the black mass. It is meaned to get the fine part, which contains only the elements (like C, Li, Mn, Ni and Co). These elements need to be in a proper quality so they can be used (re-used) in the production (construction) of new batteries.

According to the findings so far, through IBG Czech Ltd, there are currently no such comprehensive solutions, which would ensures high competitiveness.

Research highlights:

1) Li-Ion battery recycling – electric vehicles and handling equipment
2) Usage of the secondary raw materials – chemical treatment to gain elements
3) Reduction of the environmental load/ballast – usage of the gained elements
4) Competitive recycling design – production of new batteries

Dehalogenation during pyrolysis of plastics: The potential of stepwise pyrolysis in combination with metal sorbents

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Pyrolysis presents an effective solution for recycling diverse plastic waste that is otherwise difficult to process by mechanical recycling. These plastics usually contain many heterogeneous atoms such as chlorine which reduce product quality and may pose risks in the subsequent treatment of pyrolysis liquid. Therefore, dehalogenation is a crucial step of plastic pyrolysis technology. In the case of chlorine in PVC, this study proves that stepwise pyrolysis represents an effective solution that can eliminate as much as 99% of chlorine during the first heating step at 350 °C. Experiments were performed with the model plastics mixture. Also, a positive effect of the newly developed reflux extension was observed, implying a possible mechanism that when gases are allowed to expand, evolved HCl escapes the reaction zone more easily without entering secondary reactions that lead to a formation of "de novo" chlorine substances (chlorobenzene e.g.).

A concentration limit of 10 ppm of Cl, which is an allowed concentration for the introduction of pyrolysis oil into the standard oil refinery, was reached when sorbents based on $Ca(OH)_2$, and Fe_3O_4 were used in ex-situ setting. Obtained results also suggest that it is not viable to use sorbents in-situ, as it led to the increase of Cl content in the liquid. This phenomenon is not emphasized in the relevant literature.

Research highlights

1) A comprehensive study of dehalogenation of a model mixture of plastics with a high proportion of PVC.
2) Verification of stepwise pyrolysis as a key method of PVC dehalogenation.
3) Determination of the effect of different sorbent placement on dehalogenation.
4) Reaching the refinery chlorine limit of 10 ppm with novel sorbents ex-situ.

Přednáškový blok 2
(11:00 – 12:20)

Surface grafting of Mxene flakes for magnetic resonance imaging

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The unique class of two-dimensional (2D) metal carbides and/or nitrides, called Mxenes, have already shown their potential as new nanomaterials for energy storage devices, photo- and electro-catalysis, gases and ions sorption as well as for other interesting applications. [1-4]

The most studied Mxene is Ti_3C_2, which was also used in this work. The main aim of this work was to enhance the magnetic properties and response of Ti_3C_2 by grafting diethylenetriamine pentaacetate-gadolinium (DTPA-Gd) complex to Mxene surface using diazonium chemistry.

The properties, composition and structure of pristine and modified Ti_3C_2 flakes were characterized by UV-Vis, FTIR, Raman spectroscopy, XRD, XPS, SEM, HR-TEM and ICP MS techniques. The main attention was focused on the study of the magnetic properties of modified Ti_3C_2 flakes, with the utilization of temperature- and field-dependent measurements of material response and flake relaxation constants. In particular, flakes transition from dia- to paramagnetic materials was observed as a result of Gd ions entrapping. The transition from diamagnetism to paramagnetism guarantees a potential application of grafted flakes as a contrast agent in magnetic resonance imaging. Additionally, mammalian cell-based tests were also performed and indicate the low level of material toxicity, suitable for medical applications.

Research highlights

1) Modification of 2D Ti_3C_2 flakes surface for Gd ions entrapping.
2) Transition of Ti_3C_2 response from dia- to paramagnetic behaviour.
3) Application of Ti_3C_2 as a contrast agent in magnetic resonance (MRI).

References

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A microfluidic chip for cultivation of fish embryos and toxicity testing fabricated by 3D printing technology

*Petr Panuška[a], Zuzana Nejedlá[a], Jiří Smejkal[a], Petr Aubrecht[a], Michaela Liegertová[a], Marcel Štofik[a], Jaromír Havlica[a], and Jan Malý[a]

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Zebrafish (*Danio rerio*) have become a very popular animal model. They have been widely used in acute toxicity tests, the so-called fish embryo tests (FETs). Over the last years there has been an effort to develop various systems for a high-throughput zebrafish embryo cultivation and FET testing. In this work, we present a novel design of a microfluidic system fabricated by 3D printing technology and we evaluate its functional properties on *Danio rerio* embryos cultivation and toxicity testing. The development and the optimization of the microfluidic chip was performed by experimental measurements supported by numerical simulations of mass and momentum transport. The cultivation chip with two inlets and one outlet consisted of two individual channels placed on top of each other and separated by a thin partition with cultivation chambers. An individual embryo removal functionality was added to the chip design, which enhanced handling embryos in the chip. It enabled to unload any of the cultivated embryos from the chip. Long-term cultivation experiments showed a normal development of zebrafish embryos in the chip. Model toxicity tests were further performed with diluted ethanol as a teratogen. Compared to the FET assays, an increased toxic effect of the ethanol on the embryos cultivated in the chip was observed when the median lethal dose and the percentage of the morphological end-points were evaluated. We conclude that the presented 3D printed microfluidic chip is suitable for long-term zebrafish embryos cultivations and toxicity testing and can be further developed for the automated assays.

Research highlights

1) 3D printed microfluidic system suitable for zebrafish embryo cultivation and toxicity screening has been developed and successfully tested.
2) Continuous perfusion of ethanol solution results in higher toxicity for zebrafish embryos than exposure to the same concentrations under static conditions.
3) Microfluidic fish embryo test chip with a hydrodynamic-based selective single embryo removal capability has been developed and successfully tested.

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Microfluidics for exosome isolation

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Exosomes are nano-sized extracellular vesicles that carry a great potential for various fields of modern medicine. However, their wider application in research, diagnostics and therapeutics is currently limited by their small size (30–150 nm) and low concentrations in bodily fluids, meaning that time consuming procedures connected with high instrumental costs and non-negligible loss of exosomes have to be used for their isolation. Therefore, more effective means of exosome isolation are a hot topic of the last few years with microfluidic technologies promising a possible solution. [1]

Microfluidic chips for exosome isolation can be built on two basic principles, utilizing either i) immunoaffinity – based on antibodies and immune specificity of involved reactions; or ii) aiming at the physical properties of exosomes – mainly size, surface charge and density [1–3]. Even though we are at the very beginning of the research, we plan to build our chip on the principles of deterministic lateral displacement (DLD) – hydrodynamic, microfluidic technology separating particles on the basis of size in continuous flow with a resolution of down to 10 nm [4].

Our goal is to connect our experience in the fields of microfluidics and biology with the new laboratories equipped with high-end instruments for both microfluidic chips fabrication and following testing. So far, we have created several chip designs using computer-aided design (CAD) and computational fluid dynamics (CFD) and manufactured scaled-up versions of the chips using common lithography techniques and materials as a rough proof of concept.

Research highlights:

1) We have created several chip designs based on the principles of DLD.
2) We have performed preliminary CFD simulations with created chip designs.
3) We have successfully conducted initial fabrication trials.

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Methane, ethane and propane adsorption and diffusion in dual-porosity kerogens from molecular simulations

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Kerogens are organic part of shale, which otherwise consists of clay minerals, and as such they are key part in studying shale gas recovery. Shale gas, made up predominantly by methane, ethane and propane, is becoming more and more important since energy requirements of the world keep rising. Shale gas in shale rocks is partially adsorbed on the walls of the carbon kerogen backbone, which makes it difficult to extract without using stimulation techniques such as hydraulic fracturing which causes worries from environmental standpoint.

We use kerogen models developed by Bousige et al. [1], i.e., an immature marine kerogen from the carbonate-rich Eagle Ford Play, and a mature marine kerogen from the clay-rich Marcellus Play. These kerogens differ in porosity but are both only microporous, which is not sufficient to study realistic materials. Therefore, a cylindrical pore of two differing radii was added to encompass dual-porosity behaviour.

In this work we employ Monte Carlo methods to study the adsorption of short alkanes and molecular dynamics methods to study self-diffusion. We use united atom models to describe the gases and all atom model to describe the kerogens. First we utilize grand canonical Monte Carlo to determine equilibrium adsorbed amounts and thus simulate adsorption isotherms at two different temperatures. We complement the adsorption studies by simulating diffusion of the gases using equilibrium molecular dynamics and thus obtaining self-diffusion coefficients. Understanding of the properties of fluids in narrow pores found within shale is critical for identifying ways to deploy shale gas technology with reduced environmental impact.

Research highlights:

1) Realistic kerogen models were deployed and characterised to study species behaviour in those kerogens.
2) Monte Carlo method was employed to study the gases' adsorption rate.
3) Species diffusions were simulated to explore the interplay between the adsorption and diffusion.
4) Species diffusions anti-correlate with the adsorption behaviour.

References

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Přednáškový blok 3
(13:50 – 15:10)

The impact of diesel pollution on *Miscanthus x giganteus* biomass - two years pot experiment

*H. Burdová[a], K. Al Souki[a], D. Nebeská[a] and J. Trögl[a]

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Energy crop *Miscanthus x giganteus* (*Mxg*) is known for its ability to grow in contaminated soils, high biomass production as well as for the possibility to be transformed to various biobased products [1,2].

A two years pot experiment (2019 – 2020) was set to determine impact of diesel pollution on *Mxg* growth and impact of *Mxg* on degradation of diesel pollution. *Mxg* was grown in pots with diesel-spiked soil with different concentrations (2 500 – 50 000 mg/kg dry soil). Four soil samplings (three in 2019 and one in 2020) were carried out. The soil parameters (available nutrients, humus, pH, TOC) and diesel concentration (C_{10} – C_{40} analysis) were monitored. At the end of each growing season the biomass parameters (height and number of stems) were measured. After the second growing season also rhizomes and roots weight were measured. Plant fitness was quantified by measuring of leaf fluorescence. Microbial communities were characterized by respiration and enzymatic activities.

Higher diesel concentration affected negatively the growth of *Miscanthus x giganteus*. Biodegradation of diesel followed the first-order kinetics. Achieved half-lives were significantly shorter in pots with developed planted (compared to unplanted control); at low and high diesel concentrations the differences were not significant. Microbial activity was mostly stimulated by diesel concentration, which indicates microbial biodegradation as the key process. The results implicate slight stimulation of biodegradation developed by *Mxg*.

Research highlights

1) Higher diesel concentrations inhibit *Miscanthus x giganteus*
2) *Miscanthus x giganteus* increased diesel degradation
3) Diesel stimulated microbial activity

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Study of fluidized bed reactors and their use

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Plasma treatments of various surfaces are already widely used, but plasma treatments of powder materials are not so common. However, the plasma modifications of the surfaces of micro and nano particles that can potentially significantly increase their applicability. One of the solutions for particle surface treatment is a fluidized bed reactor. In particular, the plasma environment of the reactor was studied and an innovative model of the downer type fluidized bed reactor with continuous operation was designed and constructed for a larger number of modified materials.

Plasma discharge in reactor was studied by optical emission spectroscopy. Study was focused on stability of discharge, presence of individual charged particles and their intensity. Several types of materials were treated in plasma discharge and their properties were changed. Polymer powders (PE and PP) were successfully treated in purpose to increase their wettability. Increased wettability was connected with increased oxygen ratio at surface of beads and increased polar part of surface energy. In cooperation with Technical University of Liberec carbon microfibres were treated as filler in epoxy composites. Effect of plasma treatment of seeds was widely investigated. Interesting results have been achieved in the field of germination rate and speed of growth.

Research highlights

1) Downer type plasma reactor was designed and constructed
2) Plasma discharge was successfully studied by optical emission spectroscopy
3) Polymer powders had increased wettability and oxygen ratio at surface after plasma treatment
4) Plasma treatment could have positive effect on seed growth and germination rate

Iron oxide nanoparticles immobilized on activated polymer surface

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The fabrication of solid substrates with immobilized nanoparticles (NPs) on their surface is currently the subject of growing interest. The polymers are favourable as substrates because their chains are flexible. When polymer surface is activated, they contain a variety of functional groups that can efficiently immobilize NPs via molecular interactions or covalent bonds. Polymers can be easily modified to create chemically active groups or free radicals on the polymer surface by physical or chemical approaches. These activated polymer surfaces can be subsequently grafted with other chemical compounds to suit the needs for the NPs immobilization via covalent bond [1,2]. In this work, I have studied the surface properties of different polymer foils and changes of their surface properties after (i) activation by ultraviolet (UV) radiation and (ii) subsequent grafting with the iron oxide nanoparticles (IONPs). IONPs have been synthesized by co-precipitation method of ferric and ferrous ions [3]. Properties of polymers before and after individual steps of modifications were studied by different experimental techniques: X-ray photoelectron spectroscopy (XPS), contact angle measurement, and electrokinetic analysis. The success of immobilization was studied by X-ray photoelectron spectroscopy (XPS), the highest iron content was found on the polypropylene surface. We have also investigated the effect of surface pre-grafting with various compounds (e.g. chitosan, triethanolamine) on subsequent IONPs immobilization. Electrokinetic analysis showed that surface pre-grafting after UV treatment affects significantly subsequent IONPs immobilization. These findings may be of importance for advanced research and development of new materials composed of polymer and nanoparticles.

Research highlights

1) Polymer surfaces were efficiently activated by UV radiation.
2) Iron oxide nanoparticles were synthesized and successfully immobilized on polymer surfaces.
3) The highest amount of iron oxide nanoparticles was found on polypropylene surface.
4) Surface pre-grafting enhanced the subsequent immobilization of nanoparticles.

Acknowledgement

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Preferential acceleration of heavy-ions in solar flares

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We study the ion acceleration during solar flare. The solar flare is modeled using a single spontaneously fragmenting flare current sheet, which forms a plasmoid cascade. The main subject of our investigation is to determine, whether and how plasmoid cascades at the intermediate scales can impact preferential acceleration of specific ions.

The current sheet is obtained from high-resolution 2.5D magnetohydrodynamic simulations with adaptive mesh refinement (AMR)[1,2]. The ion trajectories are calculated using the test particle approach, where the background field is not influenced by particles. We use two distinct integration schemes - Vay's relativistic algorithm based on HARHA (Half-Acceleration-Half-rotation) method [3] and Guiding Center Approximation (GCA)[4,5] for analysis of individual acceleration mechanisms.

We study the energies and pitch-angles of particles, we identify the regions of most efficient ion acceleration and the main acceleration mechanisms. Influence of charge-mass ratio on ion behavior is also studied and resulting ion abundances and differential fluxes are compared with observational data.

Research highlights

1) The main acceleration mechanism is Fermi type I acceleration.
2) We observe preferential mass-dependent acceleration.
3) Abundance enhancement factors and differential fluxes exhibit power-law profiles.
4) Measured slopes for differential fluxes match observed data.

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Posterová sekce
(17:00 – 18:30)

Stop-flow microfluidic system for the immuno-capture of CTC

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Circulating tumor cells (CTCs) are rare cancer cells that are shed from the tumors into the peripheral blood and are instrumental in distant metastasis [1, 2]. The load of CTC is related to poor outcome in cancer patients and early detection of CTCs can therefore improve prognosis and help design patient-specific treatment regimes [3]. A sufficient number of these cells enable full characterization of cancer [4]. The problem is the rarity of these cells, which necessitates probing large blood volumes [3].

Here we present a dynamic microfluidic chip and evaluate conditions needed to isolate tumor cells from the cell suspension simulating blood while passing the antibody-coated surfaces of this chip. Our system enables the use of flow rather than static conditions which allows processing larger volumes of the sample in our so-called 'Stop-flow' regime. The use of an antibody-coated surface (targeting the EpCAM antigen) with a combination of fluorescence detection enables us to characterize the specific type of cancer.

The presented dynamic system is transparent, cheap to fabricate, and easy to assemble. Due to its construction and design, receptor-based cell immobilization on a large area of the substrates was optimized with a relatively small volume of antibodies. Performed tests have shown that model CTCs cell lines can be successfully captured from cell suspension mimicking blood and from processed blood on a large area of the chip.

Research highlights

1) Dynamic microfluidic chip enables the use of flow conditions.
2) The system allows processing of large volumes (ml) of the sample.
3) Model cells can be successfully captured (capture efficiency ~85 %)

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Molecular force field development for aqueous alkali halide electrolytes

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Aqueous electrolytes play an important role in many chemicals, engineering and biological processes. Yet current state-of-the-art microscopic models of alkali halide electrolytes fail to simultaneously predict thermodynamic properties of crystalline phase, aqueous solution and their equilibrium. Based on the success of our previous reparametrization of sodium chloride AH/BK3 model[1] and its excellent predictions of chemical potential of solid phase and aqueous solubility, we present extended parametrization strategy for determining ion-ion interactions of alkali halide ions. The parametrization procedure is based on a fit of lattice energy, pressure, bulk modulus and sheer modulus of crystalline phase at ambient conditions. Simple analytical approximations for the fitted properties are used in an iterative process employing simulated-annealing technique. The resulting self-consistent set of force fields (FFs) for alkali halide electrolytes is extensively tested and compared with other state-of-the-art FFs and experimental data. Simulation results show that refined FFs are able to successfully describe both crystalline and aqueous phase and their equilibrium and also accurately predict a wide range of thermodynamic and mechanical properties.

Research highlights

1) A new self-consistent set of force-fields for alkali-halides.
2) An accurate description of aqueous electrolytes by molecular simulations.
3) Straightforward, simple and general parametrization procedure for ion-ion interactions.

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Metal complexes with polyfluorinated NHCs - synthesis and biological effects

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By Finkelstein reaction we have prepared fluorinated wedge [3-(tris(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) silyl) propyl-iodide] which was used for fluorophilization of imidazole. Precursors of N-heterocyclic carbenes were prepared by quarternization. Precursors [1-methyl-3-(3-(tris(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) silyl) propyl) imidazolium-iodide] and [1-propyl-3-3(3-(tris(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) silyl) propyl) imidazolium-iodide] were converted into silver carbene complexes which were subsequently converted into other carbene metal complexes by transmetalation.

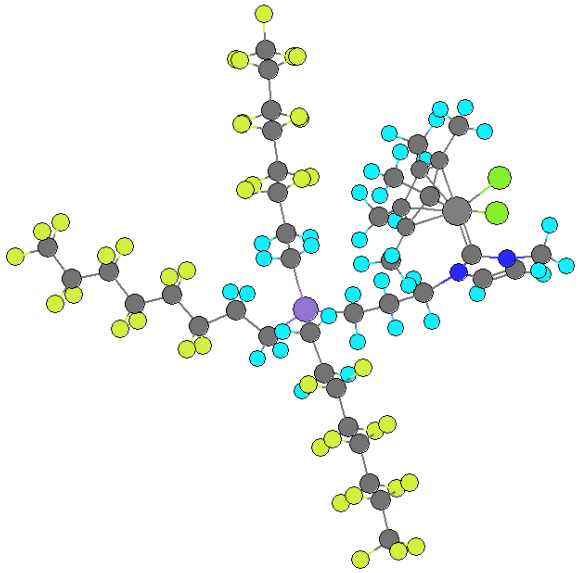

Figure 1: Cyclopentadienyl rhodium(I) NHC complexes with fluorous tag

At first we have characterized these metal complexes by multinuclear NMR spectroscopy. Properties of these amphiphilic compounds enabling their transport into living organisms will be studied, including assisted transport in the form of microemulsions, micelles or nanovesicles together with standard known amphiphilic fluorous-organic compounds. Biological activity of such compounds will be also studied on model cell cultures *in vitro* and *in vivo* on model fish *Danio rerio* as well, with the focus on study of their possible applications in biomedicine.

Research highlights:
1) Synthesis and thoroughly characterization by spectroscopic techniques (e.g. MS, NMR, IR).
2) Transport into living organisms.
3) Study of biological activities on model cell cultures *in vitro* and *in vivo* on model fish *Danio rerio*.

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Source of heavy metals in agricultural soils – man, or nature?

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Heavy metals (HM) in soil are of considerable concern to humans, and often rightly so, as some of them can be toxic (As, Hg, Cd). On the other hand, some of these metals can be micronutrients essential for plant growth, such as Zn, Cu, Mn, Ni, Fe and Co. HM can originate from the extraction and processing of ores and fly ash from industrial processes, including coal combustion, but they can also come from soil-forming rocks, especially in geologically interesting areas such as the Ore Mountains and the Bohemian Central Highlands. It is therefore often not easy to distinguish the HM origin, especially when it is usually a combination of both influences., HM concentrations are commonly determined and then compared to certain standards, if they exist at all. Alternatively, the chemically reactive fractions of heavy metals are conventionally determined as pseudo-total concentrations by chemical extraction. Either by extraction of the sample with cold 2M HNO_3, a method that better simulates the biogeochemical processes between plants and soil, or by hot aqua regia (HNO_3 + HCl), the latter being much more aggressive. However, HM reactivity is influenced by a number of factors, such as the degree of chemical weathering of rocks in the soil formation process (more mature, fine-grained soils have significantly higher extraction efficiency than immature soils or soils with high sand content, which does not necessarily mean that the fine soils are contaminated. We have gained access to the dataset from the monitoring programme of the Ministry of Agriculture (ongoing since 1990), the purpose of which was to characterise the agricultural soils of the Czech Republic in terms of the content of selected risk elements, including soil contamination, and to identify risk areas by means of pseudo-total decomposition. In total, about 60k samples are included in the database. The focus was on the safety of the food chain, analyses of agricultural soils (arable soils, pastures, and meadows), forest soils not being included. However, the results were not correlated with the geological map of the country, the composition of the parent rocks, or the total heavy metal content or elemental analyses of the soils.

This work has been conducted at a much smaller scale, a more systematic sampling and more detailed view focused only on the transect from Moldava (the Ore Mountains) to Kostomlaty pod Milešovkou (the Bohemian Central Highlands), where we try to take into account all the factors relevant for HM content, compare the results with the database of the Ministry of Agriculture and show the real anthropogenic impact on these soils.

Research highlights

1) Heavy metal concentrations are strongly influenced by local geology
2) Only detailed geochemical mapping and total elemental analysis can reveal the origin of HM
3) The Ministry of Agriculture's dataset needs a more appropriate interpretation

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Surface Modification by High-Energy Heavy-Ion Irradiation in Various Crystalline ZnO Facets

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Nowadays, self-assembled surface nanostructures on crystalline semiconductors are excellent templates for the deposition of semiconductor quantum dots and for manipulation with surface optical transparency. [1], [2] The ion irradiation with highly-energetic ions was successfully applied for modification of crystalline materials [1], [4], [5]; nevertheless, the impact of crystallographic facet on the surface morphology and optical properties of prepared nanostructures is not completely understood. In this work, we have modified the surface of *c*-, *m*- and *a-plane* single-crystal ZnO facets by high-energy W-ion irradiation with the energy of 27 MeV to observe the aspects of surface nanostructuring and the consequent evolution of optical properties. The ion fluences were kept in range $5x10^{9}$ cm^{-2} - $5x10^{11}$ cm^{-2} to see modification in the single ion regime and the regime with overlapping ion impacts. Rutherford backscattering spectroscopy in channelling regime and Raman spectroscopy identified slightly growing Zn-sublattice disorder in the irradiated samples with the progressive damage accumulation for the highest irradiation fluence, when the overlapping ion-impact regime is expected. Simultaneously, the strong suppression of main Raman modes and propagation of polar modes indicates disorder mainly in O-sublattice in the non-polar facets of ZnO. The surface morphology, analysed by atomic force microscopy, shows significant changes after the ion irradiation with a formation of small grains on the surface for *c*- and *a-plane* ZnO. The *m-plane* ZnO tends to form sponge-like surface. These surface nanostructures modify optical properties of ZnO crystal and leads to the suppression of NBE as well as DLE peaks in photoluminescence spectra and to the change of refraction index *n* and extinction coefficient *k*, determined by spectroscopic ellipsometry, which exhibits blurring of features corresponding to the particular exciton states and decrease of both optical constants in optical bandgap region.

Research highlights

1) Surface nanostructuring of crystalline semiconductors by highly-energetic ions
2) The role of ZnO facet on the defect creation and surface morphology evolution
3) The optical response of nanostructured ZnO facets

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Deposition of thin layers of covalently bound heteroboranes on PES textiles

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This communication deals with the preparation of surface-modified polymer textiles using heteroboranes with different reactive functional groups, thanks to which these substances managed to bind to some PES fabrics very tightly, by covalent bonds.

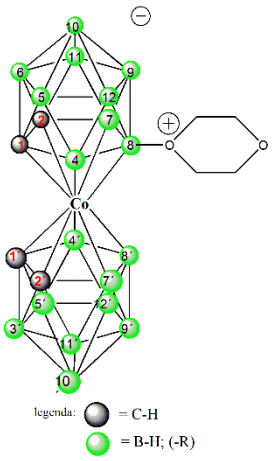

Figure 1: The heteroborane reactive block with stabilized 1,4-dioxane ring. [6]

Primary modifier, complex cobalt bis-dicarbolide anion, Cobalt Sandwich Anion (= COSAN) excels in low toxicity to mammalian cells, selective antibiofilm, antimicrobial and virostatic activity (HIV-1), excellent stability in basic and strongly acidic conditions [1-5].

Heteroborane reagents were prepared and characterized by available analytical techniques for separation and structure determination, in particular TLC, HPLC-UV-VIS, MS, NMR, EA.

In the first phase direct deposition of heteroboranes on polymer fabrics was performed, followed by removal of unreacted heteroboranes. The modified polymer fabrics were analyzed by Raman spectroscopy and XRF for the presence of cobalt. In the second phase physicochemical changes were monitored. For modified fabrics contact angles with water drops were measured. In near future tests of catalytic and possibly antibiofilm activity are planned.

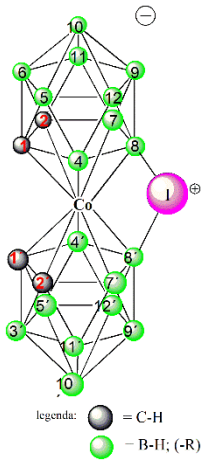

Figure 2: Another reactive heteroborane zwitterion with iodonium bridge. [7]

Research highlights:
1) Heteroborane clusters covalently attached to PES woven and nonwoven textile polymers.
2) Evidence of cobalt presence on the polymer surface.
3) Changes of contact angle of modified textiles.

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The effect of collision parameters and particle diameter on the dynamics of the mixing process by using discrete element method

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Na žádost studenta není abstrakt zveřejněn v knize abstraktů

Nutrients deficiency affects *Miscanthus x giganteus* physiology and essential metals uptake more intensively than soil contamination

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C4 perennial grass *Miscanthus x giganteus* is one of the most promising crops for phytomanagement of marginal sites which includes improvement of soil properties with energy biomass production. Two of the target types of marginal sites are localities contaminated with heavy metals and suffering from nutrients deficiency [1]. It is known from previous research that *M. x giganteus* is able to grow in such conditions, anyway it can negatively affect its physiology and concentration of metals in plant tissues which is undesirable for biomass processing [2, 3].

The goal of this study was to investigate effects of nutrients including essential metals deficiency and metals contamination on *M. x giganteus* physiology and metals uptake.

M. x giganteus plants were grown in greenhouse for two seasons in seven different real soils: two sandy soils as representatives of nutrient deficiency, garden substrate as control and four different mixtures of control soil with substrate contaminated with heavy metals by smelting industry operations. Plant physiology was examined using measurement of chlorophyll fluorescence and leaf pigment reflectance with handheld devices. Content of metals in stems, leaves and soil was determined with ICP-OES.

OJIP curves constructed from fluorescence data, same as selected fluorescence and reflectance indexes, confirmed significant stress affecting plants grown in nutrients deficient soils. Significant stress appeared also in the most contaminated soil but in variants with lower contamination, the stress level was comparable or even lower than control.

BCF (bioconcentration factor) for non-essential metals (As, Cd, Cr, Ni, Pb) was generally low in all soils which corresponds to previous observations [1]. Contrarily, BCF for essential metals (Cu, Mn, Zn) was higher than 1 in sandy soils documenting increased metals accumulation in biomass. While Cu and Mn were accumulated dominantly in leaves, Zn content was higher in stems.

Research highlights

1) Nutrients deficit is more stressful than metals contamination for miscanthus
2) Nutrients deficit stimulates uptake of selected essential metals
3) Non-essential metals are not intensively translocated to stems and leaves
4) Metals content in stems and leaves differs

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Uptake, biodistribution and elimination of carbosilane dendrimer *in vivo*

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Carbosilane dendrimers could play a key role in the field of drug delivery systems. Meanwhile, the conventional approach in therapy of oncologic, autoimmune and neurologic disease involves several of problems with side effects, the targeted drug-delivering can bring a new possibility in more gentle therapy. For effective drug delivering is necessary to test the uptake, biodistribution and elimination of used carrier in the model organism *in vivo*.

The uptake, biodistribution and elimination of fluorescently dyed dendrimer were observed in embryos of model organism *danio rerio*. We tested two ways of exposition – incubation and injection. After an exposition of 24 hours old embryos, the biodistribution was observed by a fluorescence inverted microscope for five days each 24 h. We also focused on the accumulation in a specific tissue or the possibility of elimination of nanoparticles from the organism.

In the case of incubation of intact individuals (in the chorion) the dendrimer bound to the chorion without uptake into the body. Therefore the 50μM solution was injected into the pericardial area. The distribution throughout the body was observed. Dendrimers persisted in the body throughout the observation period and no elimination mechanism appeared.

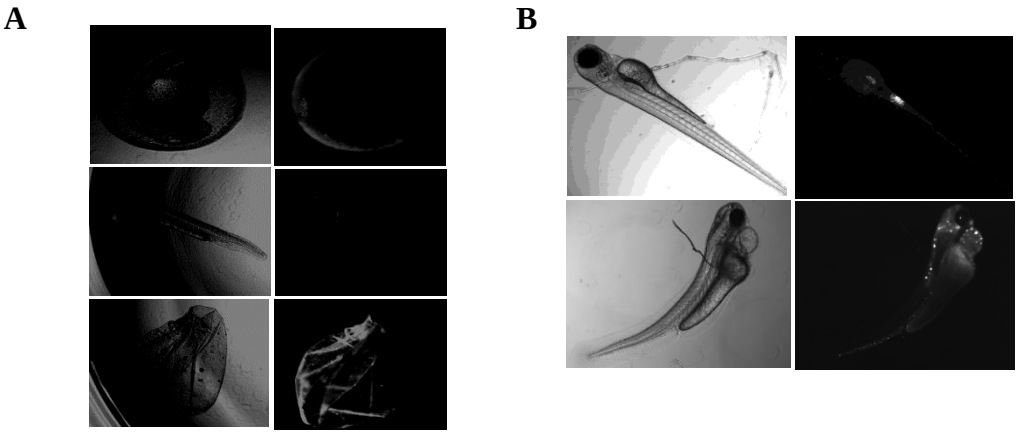

Figure 1 Micrographs of danio embryos exposed to dendrimer + Cy5 fluorescent dye. Picture A – Intact embryo incubated in 1μM solution. First and third line show the binding of dendrimer to chorion. Second line shows no uptake of dendrimer into the danio organism because of the barrier. Picture B – embryo after injection of 50μM solution of dendrimers. The fluorescent signal is present after 5 days post exposure. No mechanism of elimination from organism is observed.

Research highlights

1) The chorion acts as a very effective barrier for carbosilane dendrimers
2) For successful distribution should be dendrimer injected into pericardial area
3) No elimination of dendrimers from organism was observed
4) Dendrimer preferentially accumulates in necrotic tissue

Potential of biochar application in the phytoremediation process and biomass production of *Miscanthus x giganteus*

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The persistent increase in the contamination of soils with toxic trace elements is a serious global problem [1]. Phytomanagement has been developed as a technology to reduce and control the risk of soil contamination with toxic heavy metals, while contributing to the production of marketable biomass. *Miscanthus x giganteus* which is a bioenergy crop has been identified to be successful for phytoremediation. It has a high biomass yield which might be processed for energy purpose [2] and has the potential to be converted to other bioproducts. Miscanthus waste derived after harvesting and processing into bioproducts can be converted into biochar, a carbon-rich product via pyrolysis. Soil amendment with biochar may enhance soil quality as a soil conditioner, increase crop yield or biomass productivity as a fertilizer, and help remediate contaminated soil [3]. This research focuses on the conversion of the waste of the second generation crop *M.xgiganteus* to biochar when applied to contaminated and marginal lands, and the use of resulting biochar in impact for Miscanthus phytoremediation and biomass production. From the existing literature, the treatment processes of Miscanthus waste to produce biochar, properties of resulting biochar, and its impact on phytoremediation and biomass quantity is discussed. Results from literature assist in the determination of pyrolysis temperature and residence time for biochar preparation, and application rate for the incorporation of biochar into soil. The results show that properties of Miscanthus biochar including pH, surface area and porosity are very important in determining its impact on soil. These factors are increased with increasing pyrolysis temperature, however at very high temperatures (>700°C) properties such as surface area and porosity are reduced. Thus, an effective Miscanthus biochar will be one produced with a pyrolysis temperature of about 600°C with a residence time of about 30 minutes to an hour. Additionally, application rates of Miscanthus biochar for best impacts on soil should be between 5% to 10% (w/w). The design of the ongoing pot experiments with the incorporation of Miscanthus biochar in soil contaminated with Cu and Zn soil and its impact to the biomass production of *M.xgiganteus*, and the use of derived biochar from contaminated *M.xgiganteus* rhizomes in pot experiments cultivated with indicative *Spinacia oleracea L.* are also introduced.

Research highlights

1) Waste of Miscanthus in phytomanagement can be used as a resource
2) Miscanthus biochar supports phytoremediation process to benefit soil health
3) Miscanthus biochar may improve biomass productivity of Miscanthus x giganteus
4) Circularity of biochar use results in the efficient use of Miscanthus biomass

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Sensorics and high-resolution mass spectrometry for environmental analyses

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Presented abstract sums up major analytical progress performed during the studies. It mostly includes results outside of the present topic but significant for advancement in data quality and possibilities of high-resolution mass spectrometry (HRMS) for environmental applications. It simultaneously develops PhD competencies required for complex analytical tasks and are relevant as such. Four major subtopics will be presented.

Application and evaluation of air-quality sensors + identification of natural VOCs

Low-power and lightweight atmospheric sensors provide a wide potential for fast and flexible air quality monitoring. Their performance varies rapidly between manufacturers, therefore each atmospheric parameter was measured by different sensor to assess the most suitable ones for on-drone mount. Ammonia sensors were deployed for long-term air quality monitoring in henneries. For an exploration of natural plants VOCs, GC-HRMS identifications of *Cupressus sempervirens* and *Pinus sylvestris* headspace fingerprints was performed.

Multimethod for quantification of organic acids

Determination of organic acids is challenging by a single technique due to their various physicochemical properties. The volatile organic acids (VOAs) are most reliably quantified by direct injection of methanolic extract separated on polar column. Most of other organic acids thermally degrade before reaching boiling point, therefore their derivatization by trimethylsilyl (TMS) functional groups and separation on a non-polar column is necessary. Most of the evaluated organic acids are quantifiable on LC-DAD but with much higher LOQs.

Assessment of soft ionization for non-targeted identification by GC-HRMS

Identification of unknowns by soft ionization techniques highly depends on molecular ion yield for further fragmentation. Complexity of acquired spectra and fragment/adduct formation was assesed for three soft ionization techniques – low energy electron ionization (EI), atmospheric chemical ionization (APCI) and soft ionization by chemical reaction in transfer (SICRIT). Various standards and samples ran on each ion source for in-house database building.

Pros and cons of various quantification techniques on HRMS-qTOF

Quantification on qTOF (quadrupole – time of flight mass analyzer) may be performed by various methods. Main task is to evaluate their impact on data accuracy and discuss cost-efficiency for experiment planning.

Research highlights

1) Experiences with environmental sensorics and natural VOCs identification for on-drone monitoring
2) Implementation of methods for organic acids determination in aqueous samples by GC-MS
3) Expanding the identification capabilities of soft ionization GC-HRMS
4) Demonstration of quantification techniques for most accurate results on qTOF instrumentation

Open-source technologies in biotechnological laboratories

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Experiments in biotechnological research often require a large amount of highly specialized devices with a stable experimental environment. Many specialized devices have to be often developed by the manufacturer on demand to satisfy a customer's needs and thus comes at a high price. Many laboratories develop their own devices and willingly share a concept of their devices under open-source licenses. This sharing of concepts and plans of laboratory-developed devices can facilitate research and save finances [1].

Many of these devices such as incubators, environmental controllers, various biosensors, or even more complex devices like PCR thermocyclers or microscopes, can be easily constructed using programmable microcontrollers, sensors and 3D printed parts [2]. Specialization of these devices and their "open" hardware and software often offers its operator a bigger degree of control of the devices than the commercially sold devices, which has to serve a larger variety of applications, thus having potential of surpassing them in control possibilities.

Here we present a few of our own developed open-source devices and instruments that can be shared with other laboratories to facilitate their research. We propose a stage top incubator for long-term incubation and observation of mammalian cell lines. This incubator operates in a humid environment with a stable temperature with 0.2°C precision. Next, we present a desiccation chamber for behavioral studies of tardigrades. The temperature in this chamber can be set with the precision of 0.2°C and humidity in the range of room RH to 100% RH with the precision of 0.1% RH. The desiccation can be controlled manually or it can follow specific automatic programming. To our knowledge, no such chamber yet exists. We would also like to present a microscope stage insert for microfluidic chips, that allows their tempering with a custom-made temperature sensor of 0.01°C precision, that can be built into the fluid flow tubing. Another presented device is a rocker, where a speed, angle, and even different rocking regimes like continuous, vibrations, or fluid wave generation can be set. The last device we would like to present is a syringe pump which is currently being developed. This pump uses common plastic syringes and it is expected to be working in tandem so it should be able to achieve a semi-continuous fluid flow. Lastly, we would like to present a few small 3D printed pieces of laboratory equipment like various stands, holders, boxes, dryers and others, that improve quality of life and facilitates research.

Research highlights

1) Precise control of the environment can be easily achieved even in open-source devices.
2) The tardigrade desiccation chamber presented is the very first of its kind.
3) 3D printing can easily improve the quality of life while working in the laboratory.

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Antimicrobial effects of nanoparticles on complex microbial communities

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Nanotechnology found its way to many different scientific fields such as biomedicine, agriculture or industry. Wide usage and mass production of nanomaterials also brings up a question of their impact on nature and specifically on complex microbial communities. The activities of our research, directed to the effect of selected nanomaterials on microbial communities, have been divided into two main packages: 1) theoretical considerations based on literature review and 2) experimental works, including the preparation of methodology. Within the frame of experimental works, we have established a contact with a wastewater treatment plant and a biogas plant to acquire samples of active sludge from aerobic water purification process and samples of organic material from anaerobic digestion process. These economically valuable processes are based on participation of complex microbial communities. The change in composition of the microbial communities in both types of samples will be tested under the influence of various nanomaterials such as saccharidic and phosphonium dendrimers and TiO_2 nanoparticles. Using DNA sequencing methods, we expect to obtain a large amount of data of the sensitivity of thousands of microbial taxa. Initial cultivation experiments are directed to determinate the approximate concentration range suitable for studies of the activity of nanomaterials using sequencing methods. Our results will contribute to understanding the effects of nanomaterials on microbial communities in the environment.

Research highlights

1) Change of composition of microbial communities affected by nanomaterials
2) Possible risks for environment and natural microbial communities

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Gypsum technology of separation Li_2CO_3 from Zinnwaldite mineral

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In our modern lives we are encountering more and more with lithium ion batteries and light alloys which is the main industry of lithium consumption. World consumption of lithium has been growing steadily over the last 20 years. It's important to take an interest in this topic.

Lithium carbonate Li_2CO_3 is primary tradable raw material for the industrial production of all other lithium and is also widely used in many industries. The Czech Republic has significant reserves of lithium in the form of mica in the mineral zinnwaldite. The total reserves of ores with increased lithium content at Cínovec were estimated to have least 300 Mt with an average metal content of 0.117% Li.[1]

Lithium mining took place in Cínovec already in the years 1953 to 1967. Was produced a total of 23 kt of Li concentrate, which was processed at the Lachema Kaznějov chemical plant. Due to high transport costs, the continuation of mining was abandoned.

Several technologies of zinnwaldite concentrate processing have been developed at the Research Institute of Inorganic Chemistry in Ústí nad Labem. The best yield was shown by the gypsum method based on thermal sintering of the concentrate with a $CaSO_4$ and $Ca(OH)_2$.

Due to the rising price of lithium carbonate, mining at Cínovec will be resumed maybe, but it also broughting certain problem. Today is only one active mine for natural gypsum in Kobeřice near Opava in the Czech Republic. This represents a long transport distance of the raw material of 450 km. In addition, the $CaSO_4$ content of the raw material is only 66% and the rest is made up of clays.

Therefore, it would be appropriate to replace natural gypsum from lalternative sources. Because Zinnwaldite deposits are located in Northern Bohemia, where since most of coal-fired power plants in Czech Republic are located it's our best option to try use energy gypsum. As we know during the desulphurization of their flue gases, a practically unlimited amount of energy gypsum is produced, which is sold cheap as certified raw material.

The aim of my research is to modify the original gypsum method for the use of energy gypsum. First, I will compare the chemical composition of energy gypsum samples from different coal-fired power plants and select the most suitable one, which will be used as an alkaline additive in the melting of zinnwaldite concentrate and test while maintaining the same technology parameters as for natural gypsum. If the reactions willnot be proceed as expected, I will adjust the ratios of the molten components, melting time or temperature.

The melting batch consists of zinnwaldite concentrate, energy gypsum $CaSO_4$. $2H_2O$ and $Ca(OH)_2$ in a ratio of 6:4,2:2 and is melted for 60 minutes at 950 °C. The resulting clinker is ground, dissolved and leached in water. The composition of the obtained sulphate extracts allows their simple and effective purification. Using potassium carbonate, it is then possible to precipitate relatively pure Li_2CO_3, which is suitable both for sale and direct use in industry, and for the production of lithium compounds, including high-purity Li_2CO_3.[2]

Research highlights

1) Lithium carbonate
2) Gypsum technology ofseparation Li_2CO_3fromZinnwalditemineral
3) UtilizationofZinnwalditeWastesforRecoveryof Lithium
4) Li concentrate from waste raw materials generated during the separation of tin and tungsten

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Interaction of pollutants on nanoceria

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Cerium oxide is a relatively widespread material with many applications in the industry, it is also an important heterogeneous catalyst. Cerium oxide may be prepared in nanocrystalline forms then is usually so-called nanoceria. Low-temperature synthesis for the preparation of active forms of nanoceria have been previously optimized at the workplace of UACH[1]. This form has the ability to decompose highly toxic compounds such as organophosphorus pesticides[2]. Applications of nanoceria emerge in biology, biochemistry and biotechnology thanks to the pseudoenzymatic properties of CeO_2 [3] associated with the decomposition of the phosphoester bond[4].

Removal of toxic chemicals from wastewater remains one of the most important subjects in pollution control[5]. By using non-toxic material (such as nanoceria) to mitigate contaminants of emerging concern helps avoid their further spread. And that's also because clean water is a key challenge identified in the UN sustainable development goals.

This contribution is focused on expanding the portfolio of known environmental pollutants that can be decomposed or at least sorbed on the surface of nanoceria. A significant motivation is to help to look for ways to reduce the total amount of hazardous substances in the environment. The interactions of nanoceria with more than a hundred environmentaly relevant substances have been studied. These substances are usually used as pesticides or medicines.

Research highlights

1) Optimized synthesis of uniform CeO_2 nanoparticles under ambient conditions in water
2) Expansion of the portfolio of substances interacting with CeO_2
3) Comparison of decomposition kinetics for different groups of pesticides
4) Proof of physisorption for common drugs

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Biodistribution and cytotoxicity of phosphonium carbosilane dendrimer

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Drug delivery systems are engineered technologies in which an active compound is packed into or loaded on a biocompatible nanoparticle. Dendrimers (DDMs) have demonstrated great potential for targeted therapy due to their shape, defined size, the presence of the void space and molecular weight. Here we report biodistribution and cytotoxicity of phosphonium carbosilane dendrimer with $P(C_6H_4\text{-}OMe)_3$ peripheral substituent. This work uses 3D multicellular tumour spheroids to assess *in vitro* distribution and toxicity of the carbosilane dendrimer. For spheroids formation, a commercial 3D Petri Dish® was used. Cytotoxicity was tested by CellTiter-Glo® Luminescent Cell Viability Assay. The $P(C_6H_4\text{-}OMe)_3$ dendrimer was labelled using fluorescent photostable, cyanine dye (Cy5). Biodistribution of dendrimer-Cy5 conjugates (D-Cy5) was investigated through microscopy imaging and confocal microscopy. Spheroids for confocal microscopy were stained with a mixture of Hoechst 33342 and Mitotracker Red. The optimal concentration of carbosilane dendrimer for biodistribution monitoring was established. D-Cy5 was mainly accumulated in the periphery (proliferating zone) of spheroids at 24 h. After 72 hours, D-Cy5 was detected in mitochondria. Phosphonium carbosilane dendrimer with $P(C_6H_4\text{-}OMe)_3$ peripheral substituent could be valuable for gene therapy applications due to relatively low cytotoxicity, the presence of positive charge for nucleic acid electrostatic binding and high potential of mitochondrial targeting.

Research highlights

1) The optimal concentration of dendrimer for biodistribution studies has been determined.
2) The dendrimer accumulation in mitochondria was confirmed.
3) A fast and simple method for observing the spheroid core has been introduced.
4) The distribution of dendrimer was determined by confocal microscopy.