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Faculty of Environment

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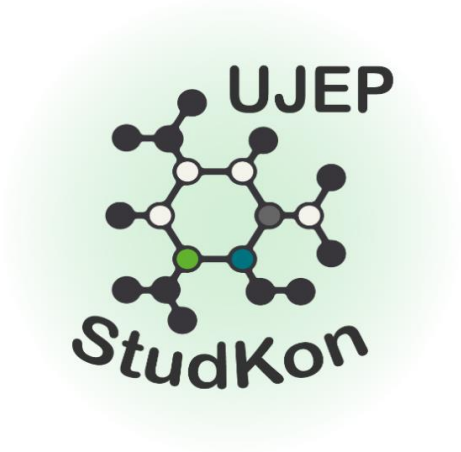
Faculty of Science



BOOK OF ABSTRACTS

5th Conference of Natural Sciences and Technical PhD study programmes at UJEP

StudKon 2022

13. 6. 2022

Green Lecture Hall (Multifunctional centre at UJEP Campus)

J. E. Purkyně University in Ústí nad Labem

http://www.studkon.ujep.cz

Conference Programme

MONDAY 13. 6. 2022 / Green Lecture Hall (Multifunctional centre at UJEP Campus)	
Registration	**8 – 9 a.m.**
Morning sessions	**9 a.m. – 1:20 p.m.**
9 – 9:10 a.m.	Opening and welcome session
9:10 – 10:30 a.m.	Talks session 1 9:10 Slavomír Adamec 9:30 Katrien Boonen 9:50 Robert Ato Newton 10:10 Eva Štěpanovská
10:30 – 11:00 a.m.	Coffee break
11:00 a.m. – 12:20 p.m.	Talks session 2 11:00 Michaela Průšová 11:20 Kateřina Přibylová 11:40 Anna Paříková 12:00 Martin Kozakovič
12:20 – 1:20 p.m.	Lunch break
Afternoon sessions	**1:20 – 7:00 p.m.**
1:20 – 1:40 p.m.	Short poster presentations
1:40 – 3:00 p.m.	Talks session 3 1:40 Jakub Tolasz 2:00 Pavel Kaule 2:20 Petr Aubrecht 2:40 Dominik Pilnaj
3:00 – 3:30 p.m.	Coffee break
3:30 – 4:30 p.m.	Prof. Petr Svoboda: Tři hlavní akademické hrdelní zločiny - plagiarismus, falsifikace a fabrikace (in Czech)
4:30 – 6:30 p.m.	Poster session
6:30 – 7:00 p.m.	Technical break
Evening programme	**7:00 – 10:00 p.m.**
7:00 – 7:30 p.m.	The M. Broul award ceremony – **Auditorium CPTO 1.03**
7:30 – 10:00 p.m.	Barbecue

TALK SESSIONS

TALK SESSION 1 (9:10 – 10:30 a.m.)

9:10 a.m. **Slavomír Adamec**: Risk elements in soils in selected areas of northwestern Bohemia

9:30 a.m. **Katrien Boonen**: The potential of dendrochemistry in pollution research

9:50 a.m. **Robert Ato Newton**: Fuel characteristics of Miscanthus x giganteus biomass produced at the marginal and slightly contaminated by trace elements soils

10:10 a.m. **Eva Štěpanovská**: Nanostructuring in carbon-based materials and polymer composites by energetic ion beams to improve electrical and sensing properties

TALK SESSION 2 (11:00 a.m. – 12:20 p.m.)

11:00 a.m. **Michaela Průšová**: Isolation and characterization of plant exosomes for biomedical applications

11:20 a.m. **Kateřina Přibylová**: Study of transport properties of PEBAX 1657 and PEBAX 2533 membranes

11:40 a.m. **Anna Paříková**: Particle transport in microfluidic devices: a multiscale modeling approach

12:00 noon **Martin Kozakovič**: 1D Model of a heat and mass transfer in a rotary kiln

TALK SESSION 3 (1:40 – 3:00 p.m.)

1:40 p.m. **Jakub Tolasz**: Interaction of pollutants on nanoceria

2:00 p.m. **Pavel Kaule**: Heteroboranes metallacomlexes for homo- and heterogeneous catalysis of esterification

2:20 p.m. **Petr Aubrecht**: Development of a nano/microstructured functional materials and microfluidic devices usable for bioapplications

2:40 p.m. **Dominik Pilnaj**: On-line sensorics and high-resolution mass spectrometry for tropospheric monitoring

POSTER SESSION

4:30– 6:30 p.m.

Akintoroye Mayowa	Comparing the impact of different biochar concentration on wastewater treatment
Gabriela Bílková	Factors controlling manganese concentrations in the leaves of silver birch (Betula pendula Roth) in relation to recent acidification of mountain forest soils of central Europe
Hana Burdová	Characterization of pyrolysis oils by GC(xGC)-FID/HRMS
Šárka Dědičová	Effect of electric field on the structure of polymer solutions
Tereza Dušková	Metal complexes with polyfluorinated NHCs - synthesis and biological effects
Kristína Fiantoková	Obtaining of the active mass from the spent Li-Ion batteries
Jakub Hoskovec	Electrospun membranes chemically modified for hydrogen and carbon dioxide capture
Jan Hubáček	Pyrolysis of plastics: Dehalogenation via stepwise pyrolysis and metal sorbents
Adéla Jagerová	Preparation of Au nanoparticles by energetic ion beams in crystalline GaN
Michaela Kocholatá	Isolation and characterization of plant exosomes for biomedical applications
Pavlína Matysová	Molecular simulation of salt hydrates
Viktorie Neubertová	Covalent functionalization of MXene flakes for stable and biocompatible MRI contrast agent
Petr Panuška	All-in-one OSTE+ droplet microfluidic tumor spheroid chip
David Poustka	Microfluidic Tissue Barriers
Eliška Rezlerová	Shale gas and carbon dioxide adsorption and diffusion in dual-porosity kerogens from molecular simulations
Michal Syrový	Chemical modification of PAN – based nanofibrous membranes prepared by electrospinning and their properties for CO_2 capture potential
Jan Štěpka	Analysis of the effect of CeO_2 nanoparticles on microbial communities in wastewater treatment process
Martin Šulc	Gypsum technology of separation Li_2CO_3 from Zinnwaldite mineral
Zuzana Žmudová	Expression of multiple galectins in glioblastoma cell lines and exosomes

ABSTRACTS

Risk elements in soils in selected areas of northwestern Bohemia

Slavomír Adamec[a*]

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My PhD work will deal with the pollution of soils in the NW Bohemia with risk elements with special emphasis on As, Be, Cd, and Sb, as well as organic pollutants, especially polycyclic aromatic hydrocarbons (PAH) produced by coal combustion. The area of northwestern Bohemia was chosen both for its great geological diversity and also for its changes caused by extensive anthropogenic activities in the past. Agricultural land in that area has elevated concentrations As and Be, however, it is not clear if these have resulted from anthropogenic contamination or from natural anomalies in the bedrock. Contamination of NW Bohemia can come from both ore mining and processing and coal mining and combustion. In the case of coal mining and utilization, contamination by atmospheric fallout (As, Cd, Sb) could have occurred in a diffuse manner over vast areas and regardless of the bedrock, while contamination from ore mining and processing (As, Sb) can be expected to have smaller spatial impact around historical mines and smelters; both should increase upward in soil profiles. Geogenic anomalies should result in association of elevated concentrations with geological units and be homogenous in soil depth profiles. The analysis of organic pollutants will serve as a proxy for the impact of coal combustion in the area and the approximate dating of sediments.

So far, several soil profiles have been sampled in the Teplice region and in the Ore Mountains. In 2021, samples were taken in 10 depth profiles from depth of 0 - 100 cm with 20 cm increment. In 2022, one soil profile and ca. 20 pairs of top (10 cm) and bottom (40 cm) soils samples were taken in the Ore Mountains in 6 bedrock geologies. Ca 10 soil profiles will be sampled in the lowland in the Teplice Area and reference locality NW of Lovosice. The analytical methods in this work include acid extractions and analysis by ICP-MS, HPLC-MS as well as total analyses by XRF. Analyses show that many samples in the study areas have elevated arsenic concentrations, that up to now seems to point to geogenic control. The aim of the work will be to distinguish natural contamination from the bedrock and the consequences of anthropogenic activities in this year.

Research highlights

1) Soil contamination in northwestern Bohemia is related to the great geological diversity and anthropogenic pollution in the past.
2) It is important to distinguish between natural geogenic and anthropogenic contamination for the use of agricultural land.

Comparing the impact of different biochar concentration on wastewater treatment

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The objective of the this research is to examine the effect of different biochar concentration on contaminant removal in wastewater. In recent years biochar has been discovered to be a suitable pharmaceutical contaminant removal.

In this research, it was examined if biochar is suitable for the treatment of pharmaceutical contaminants in wastewater, different contaminants was examined with different biochar concentration and it was discovered that biochar might not be able to remove all pharmaceutical contaminant from wastewater, it is still effective in the reduction of the concentration.

For instance, acetebulol which was one of the contaminants found in wastewater sample collected was found to be about 184ng/l before treatment, and 84ng/l for 0.1g biochar treatment, 60ng/l for 0.25ng/l and 41.6ng/l for 0.5g biochar treatment.

The research will continue with the application of the treated wastewater in soil and plants, specifically rye grass to examine if the pharmaceutical contaminant are transferred to soils and plants respectively.

Research highlights

1) Wastewater samples was collected from WWTP north bohemia region
2) Pharmaceutical contaminants of different concentration was found in the wastewater
3) Wastewater was treated with different biochar concentration
4) Biochar is effective for wastewater with pharmaceutical contaminants.

Development of a nano/microstructured functional materials and microfluidic devices usable for bioapplications

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With the Covid-19 outbreak, there is an increased demand for complex and affordable diagnostic and medical devices capable of interactions with biological entities such as cells, viruses, or proteins/antibodies. Microfluidics is an extremely useful tool that provides this capability and can mimic complex biological systems [1]. But to this day it remains more of a tool for researchers and most of the designs of lab-on-chip systems never reaches beyond a proof-of-concept prototype and it is seldomly followed by commercial product [2]. The main reason is that there is a lack of consistent material, fabrication, and interfacing technology [3].

Here we present a set of technologies that combines a novel material OSTE+ with soft-lithographic techniques. Soft-lithography is the go-to technology for rapid prototyping of microfluidic devices but still needs hard masters with well-defined nano/structures. We optimised the processes for photolithography and reactive ion etching for the preparation of hard masters (etched silicon and with SU-8-based resist) for soft-lithography.

We are able to use these masters not only with PDMS but also with the OSTEMER a novel material (ternary system consisting of thiol, allyl, and epoxy monomers) specifically developed for use in microfluidics [4]. The OSTE+ as a manufacturing platform shows several key advantages such as tuneable mechanical properties, tuneable surface properties allowing permanent surface modifications of specific regions; adhesive-free room-temperature bonding to glass, silicon, plastics, and itself; ease of manufacturing including UV-curing and photopatterning and biocompatibility [4]. With this set of tools, we are capable of creating advanced microfluidic devices such as organs-on-chip.

Research highlights

1) Hard technologies optimised for the creation of fine structures up to micrometre scale
2) Combined with soft-lithography and 3D printing for rapid prototyping
3) Use of a novel material OSTE+ specifically designed for microfluidics
4) Set of tools for fabrication of complex microfluidic devices e.g., organs-on-chip

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Factors controlling manganese concentrations in the leaves of silver birch (*Betula pendula* Roth) in relation to recent acidification of mountain forest soils of central Europe

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Manganese concentrations in leaves of silver birch (*Betula pendula* Roth) were studied in the Ore Mountains and several reference localities in Bohemia, both mountainous (up to 950 m MSL) and lowland (ca. 300 m MSL). The studied mountainous areas have been seriously damaged by acid rains in the last decades and forests there have still not recovered from that crisis. The focus of this work is to understand this state and describe mechanisms that control the uptake of unwanted metals by plants. Geology and the content of other elements (especially Mg) play an important part in the Mn accumulation by birch. The largest excess of Mn was found in Mn rich and Mg poor soils, that are expected to be particularly prone to acidification.

This work is a continuation of the previous research of E. Kula, but from a different point of view. Our current work focuses on environmental geochemistry and examines the influence of bedrock geology, soil acidity and nutrient imbalances on Mn uptake by plants. One of our current goals is to use Mn concentrations in leaves of birch as possible proxy for recent acidification of mountain soils.

Sampling in Czech Republic (Bohemia and Moravia) will be supplemented by sampling in selected localities in Germany to decide whether the Ore Mountains are anomalous in the Central European context. In addition to birch, other tree species will be studied, probably common beech and rowan. It is possible that different tree species have different strategies to deal with excess bioavailable Mn and nutrient imbalances.

Among other goals, our future work will verify the applicability of the portable XRF to analyse Mn concentration in whole leaves directly in the field. This could serve as a tool for preliminary analysis of local variability and we expect it will save a lot of time in field.

Research highlights

1) Environmental geochemistry of anthropogenically disturbed soils
2) Distinguishing between geogenic and anthropogenic influences
3) Why are the forests in the Ore Mountains still so damaged?

The potential of dendrochemistry in pollution research

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Dendrochemistry is the science of analysing chemical variations in tree rings as a proxy for changes in the environment [1]. One of its applications is the investigation and dating of past pollution events. Before trees can be effectively used as pollution archives, however, some issues need to be better understood. Pollutants are not necessarily kept in the ring of the year they were taken up by the tree, but can be moved through the bole wood [1]. This translocation of chemicals depends on tree physiology and structure and the properties of the chemical substance [1]. There are indications that a high number of rings in the sapwood, the physiologically active part of the xylem, promotes the translocation of pollutants [2]. One goal of this research is to evaluate whether sapwood thickness is an indicator of the suitability of a tree species for dendrochemistry.

We aim to measure pollutants in the structural substances of the cell walls, as the non-structural substances can vary with season and stage of heartwood formation [3]. Extraction could reduce the influence of non-structural substances such as xylem sap, resins, and heartwood substances [3]. Therefore, a preliminary experiment was carried out to determine whether extraction with deionised water is a useful pretreatment of larch cores. Extraction was done by soaking the core at room temperature for three days or by placing it in an ultrasonic bath. We focused on mercury, since Hg in tree rings is a promising indicator of Hg concentration in the atmosphere [4]. Hg was analysed by cold vapour atomic absorption spectrophotometry using an Advance Mercury Analyzer (AMA 254). The larch samples taken in Ústí nad Labem had a relatively high Hg content, thus it was possible to measure Hg per annual ring or two-year section. Even the untreated core did not show the expected effects of the xylem sap, possibly because the Hg content of sap was low and little sap was present, as samples were taken early in spring. Therefore, we cannot conclude if the pretreatments effectively remove the xylem sap. Soaking reduced the weight of the samples by dissolving hydrophilic extractives in the heartwood, and hence increased Hg concentration.

Research highlights

1) Measuring Hg in each annual ring of larch offers a high-resolution result.
2) Soaking larch cores in deionised water reduced the weight of the heartwood.
3) Soaking could potentially be useful as a pre-treatment to remove extractives.

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Characterization of pyrolysis oils by GC(xGC)-FID/HRMS

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Pyrolysis oils (PO) have aroused interest recently, as they are liquid energy carriers and alternative source of chemicals in petroleum and chemical industry. They are complex mixtures of hundreds of components and chemical compounds. Their composition depends mainly on the input material (e.g. plastic waste, sludge, tires, biomass). The detailed structural analysis of the oils is essential for their efficient use and optimization of a pyrolysis process. One- or two-dimensional gas chromatography in combination with high resolution mass spectrometer (HRMS) provides selectivity, which is crucial for non-target compound identification.

Innovated qualitative and quantitative GC-MS methods for characterization of pyrolysis oils (including halogenated compounds from pyrolysis) were developed. They will be presented within this contribution, together with their optimization, validation and examples of analyses of real pyrolysis oils.

Research highlights

1) Innovated qualitative analysis of pyrolysis oil by GC-HRMS
2) Group characterization of pyrolysis oils (GCxGC-FID/HRMS x GC-FID/HRMS)
3) Qualitative and quantitative analysis of halogenated compounds from pyrolysis

Effect of electric field on the structure of polymer solutions

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The interaction of polar molecules with an external electric field provides a tool for manipulating molecular structure. And this is also the case for polar polymers, which can undergo complex structural changes due to the external electric field. The study of such changes in the polymer structure is of great importance, for example, for the technology of electrospinning. The microscopic changes caused by the electric field influence both the quality of the electrospinning process and the properties of the resulting materials. The effect of electric field on the structure of polymer chains can be studied experimentally, theoretically or by methods of molecular modeling. In previous molecular modeling studies [1, 2], special attention was paid to modeling the dynamics of the initial stages of the process of electrospinning of polymer solutions. In this contribution, our recent molecular dynamics simulation study [3] is extended by including short ethylene glycol oligomers. In an effort to explain the results of work [3], molecular dynamics simulations are carried out to study the structure of mono-, di-, tetra- and octaethylene glycol in water and methanol. The field-induced structural changes of the oligomer molecules in both solvents are monitored and used to infer what might be responsible for the solvent specific, field-induced anisotropy of a polymer coil reported previously [3].

Research highlights

1) Perform molecular dynamics of ethylene glycol oligomers in polar solvents.
2) Identify structural changes of an oligomer molecule induced by an electric field.
3) Describe the effect of the electrostatic field intensity and chain length on studied changes.

References

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Metal complexes with polyfluorinated NHCs - synthesis and biological effects

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Due to the increasing needs of the industry the environmentally friendly synthesis process is an important objective. Most research is based on reworked or new developed methods. Fluorous chemistry allows easy separation of the product and reusable solvent use.[1]

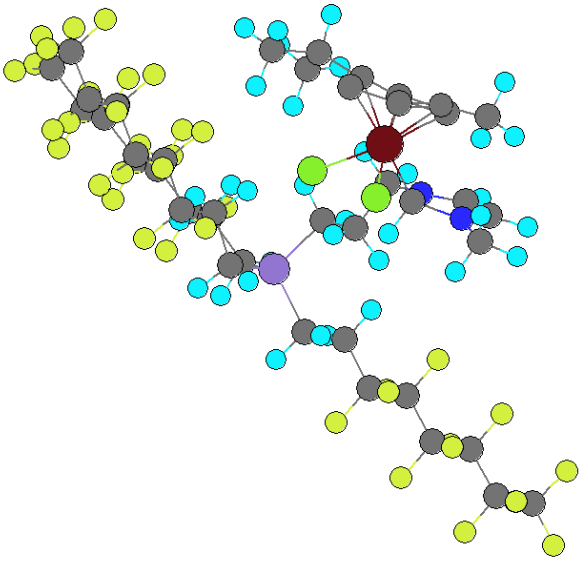

Figure 1. P-cymene ruthenium(I) NHC complex with fluorous tag

Several transition metal complexes of NHC ligands bearing polyfluoroalkyl tag were prepared by standard transmetalation proceedure.[2] At first all of these metal complexes were characterized by HRMS, EA and multinuclear NMR spectroscopy. Immediately it was apparent that all the complexes were chiral.

Fluorous tag allows use of metal complexes in two phase catalysis. Thus, metal complexes could be used under homogenous catalysis conditions and later separated. 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.[3]

Research highlights

1) Study of activity of metal complexes in two-phase catalysis system, e.g in transfer hydrogenation.
2) Racemization study at various temperatures.
3) Study of biological activities on model cell cultures *in vitro* and *in vivo* on model fish *Danio rerio*.

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Obtaining of the active mass from the spent Li-Ion batteries

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As the demand for electric vehicles (EV, EVs) rises, rises also the demand for raw materials which are crutial for the production of the Li-Ion batteries (LIBs, LIB), thanks to which are the EVs powered. As the push on recycling is rising, also the prices for the raw materials itself, and the thoughts of independency from the Asian market, the concepts of Gigafactories comes in mind. However the construction of the LIBs can be complicated as it consists from several different parts, metals and elements. Nevertheless the focus on the environment and the protection of the planet should play a higher role in our basic life.

Nowadays, there are several possibilities how the LIBs can be recycled, e.g. pyrometalurgical or hydrometalurgical treatments. There is also a way, which is called as a Direct Recycling (DR). One of the possible DR processes has been described, on the laboratory scale, by *Xiaoping Fan et all* in the article „*Separation and recovery of valuable metals from spent lithium-ion batteries via concentrated sulfuric acid leaching and regeneration of* $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$“. Based on the described conditions there have been several experiments made, that proved the possible application in a pilot plant.

Usage of the sulfuric acid (H_2SO_4) for the removal of the polyvinylidene fluoride (PVDF), which is used as a glue that holds the aluminium foil (Al foil) and the active mass (NMC – Ni, Mn, Co) together, is very effective, but only when it comes to high concentration. By low concentration the leaching effect is small and it needs to be supported by manual removal of the active mass. Afterwards has been the hydrogen peroxid (H_2O_2) used, which has several effects: i) separation of the Al foil from the active mass (NMC – Ni, Mn, Co) and flotation effect, ii) reduction effect, which changes the oxidation number of the elements, that is needed for the stepwise precipitation.

Thanks to the ICP-MS analysis, the observation of the experiments and calculating, it can be said that the removal of the PVDF is effective, by the 18M H_2SO_4 roughly 95,4%, by 16M H_2SO_4 90,1%, by 8M H_2SO_4 93,6% and by the 4M H_2SO_4 64,8%. By the lower concentrations, like 8M and 4M H_2SO_4, is the effect low and the PVDF is being removed only partialy and the loosened NMC was supported by manual removal, and therefore these dilutions are not recommended for usage, as there is still a lot of NMC left on the Al foil. Therefore the process, as described in the article, can be applied, but not fully and needs to be modified when wanted to be applied into the pilot plant.

Research highlights:

1) Li-Ion batteries
2) Recycling process – designed recycling
3) Described conditions and their modification – possible application in a pilot plant
4) Usage of the grained materials – recycling as a part of the concept of Gigafactories

Electrospun membranes chemically modified for hydrogen and carbon dioxide capture

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Electrospinning technology was used in a one-step and multi-stage process for the development of modified polyurethane nanofiber membranes (PUR) for targeted capture of selected components of pyrolysis gas - hydrogen (H_2) and carbon dioxide (CO_2);

First, a multi-stage process with modifying substances in the form of palladium and platinum nanoparticles was used for targeted H_2 sorption. Chloride salts of said metals and hydrazine were used as reducing agents for the synthesis of these nanoparticles. The reaction took place directly in the spinning solution, where PUR was deposited as a steric stabilizer.

Second, selected amines triethylenetetramine (TETA) and tetraethylenepentamine (TEPA) were used to capture CO_2 in a one-step process.

The samples were characterized by a number of analytical and testing methods, for example to investigate surface chemistry, Zeta potential, structure, morphology, phase composition, mechanical properties, sorption capacity, etc.

The results of all tests revealed the influence of technological parameters on the main studied parameter of sorption capacity, which is crucial for the design of functional units working as a H_2 and CO_2 trap. The results are especially useful for finding relationships: technology - structure - properties that are important for the design of a membrane with maximum sorption capacity maintaining air permeability, necessary for a membrane capturing selected components of pyrolysis gas.

Research highlights

1) Successful incorporation of 4-12 nm nanoparticles into the nanofiber membrane.
2) The highest achieved value of sorption capacity for CO_2 was 13.97 cm^3/g.
3) Influence of technological parameters on sorption capacity.

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Pyrolysis of plastics: Dehalogenation via stepwise pyrolysis and metal sorbents

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Pyrolysis is a perspective way of recycling plastics into virgin polymers. However, due to the variety of plastic types and included additives, the pyrolysis of plastic waste is a complex process that yields different quality products. In order to process pyrolysis products into new polymers, it is necessary to remove halogens, especially Cl and Br, that may cause corrosion of technology, inactivation of catalysts, and deterioration of products. This study aimed to understand the dehalogenation mechanisms and achieve dechlorination of liquid products from a model plastic mixture containing PVC. Different pyrolysis settings and sorbents were used to decrease the Cl content below the set limit of 10 ppm. It was observed that it is not feasible to use sorbents directly in the reactor (in-situ) as the captured Cl is released over higher temperatures yielding even more Cl in the products. Introducing the step at 350 °C (stepwise pyrolysis) proved to be a crucial part of the process. The introduction of reflux extension provided unexpected dehalogenation by decreasing the time of HCl in the hot reaction zone. Required Cl content was reached via a combination of stepwise pyrolysis, reflux extension, and sorbents ($Ca(OH)_2$, Fe_30_4-Si) in a separated bed (ex-situ) at 300 °C. Results have direct implications for designing an efficient pilot plant or modifying current technologies without a dehalogenation procedure.

Research highlights

1) In-situ sorbent placement led to an increase in chlorine content in liquid products.
2) Novel reactor extension improved the yield of liquid products and chlorine content.
3) 3-23 ppm of Cl was reached by combining stepwise pyrolysis and sorbents ex-situ.
4) Fe_3O_4 and $Ca(OH)_2$ were efficient for dehalogenation at 300 °C.

Preparation of Au nanoparticles by energetic ion beams in crystalline GaN

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Crystalline GaN is a wide direct bandgap (3.4 eV) semiconductor applied in high power electronics or in optoelectronic devices working in UV wavelength region such as blue LED and detectors. [1,2] The modification of GaN with Au nanoparticles (NPs) can increase absorption of visible light and, therefore, extend GaN application to this region. [3] The ion implantations can be used for the preparation of metal NPs in solids without any chemical reactants exhibiting high purity of NPs or good control over the NPs depth distribution. However, ion implantation leads to implantation damage which may affect material properties, especially in the case of crystalline material implantation. [4] We implanted *c-plane* GaN crystals with 1.85 MeV Au ions with fluences in the range of 1.5×10^{16} cm^{-2} - 7×10^{16} cm^{-2} to prepare Au NPs and study the optical response of the prepared structures. To support the growth of Au NPs and induce GaN structure recovery, implanted samples were annealed at 800 °C in ammonia atmosphere for 20 minutes. The Rutherford backscattering spectroscopy in channelling mode was applied for elemental composition analysis and structural characterisation before and after annealing. Samples implanted with lower ion fluence shows Gaussian distribution of the implanted Au ions. An increase in implantation fluence leads to the shift of Au ions towards the surface and the creation of multimodal depth profiles of implanted Au ions accompanied by the appropriate development of disorder depth profiles. Post-implantation annealing leads to partial structure recovery and causes strong Au-ion redistribution connected to the growth of Au NPs as it was confirmed by transmission electron microscopy (TEM). TEM also shows distinct stages of Au NPs formation for particular ion-implantation fluences after annealing in connection to GaN radiation damage evolution during Au-ion implantation. Additionally, the plasmonic behaviour of the created Au NPs was observed by photoluminescence (PL) analysis exhibiting new signal at the wavelengths around 500 nm and change in diffusion reflectance, mainly in the spectral range of 500 – 600 nm, where the Au NPs enhances absorption and scattering efficiencies for photons.

Research highlights

1) Preparation of Au nanoparticles in crystalline GaN by ion implantation
2) Evolution of Au nanoparticle formation and radiation damage in GaN
3) Distinct plasmonic behaviour of prepared GaN/Au NPs layers

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Heteroboranes metallacomlexes for homo- and heterogeneous catalysis of esterification

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This communication deals with the preparation of variously substituted heteroborane clusters for their use in hetero- or homogeneous catalysis of fatty acid esterification with bioethanol with a high degree of sustainability. It have been described the substances among class of carboranes that excel in superacid behavior [1].

The main purpose of this work was to prepare derivatives using Cobalt (bis) dicarbolide anion[2]. The aim was to prepare tetra C-halogen substituted derivatives, which would excel especially in high stability. After many experiments were indeed prepared the original derivatives, but the XRD analysis show they were still substituted on the boron atoms. However, these substances have been used as homogeneous catalysts in the esterification of FA. The second partial goal was to anchor the heteroborane analogues on a solid carrier, forming thin layers by covalent bonding. They were chosen two heteroborane zwitterionic complexes[3,4] and textile polymers were selected as substrates for the preparation of these modified materials.

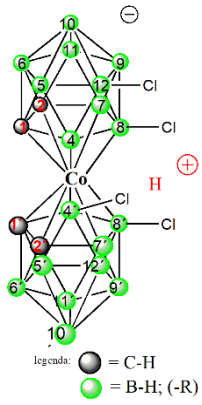

Figure 1: The structure of tetra chlorine COSAN acid.

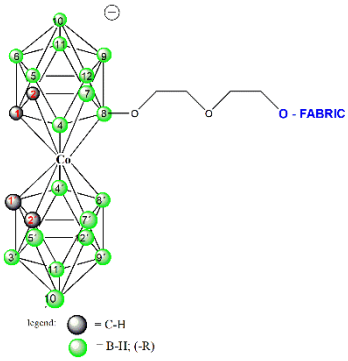

Figure 2: The scheme of deposition of heteroborane compound on the surface of textile fabric.

The first step was always the synthesis of the heteroborane conjugate with the characterization by advanced analytical methods (e. g.: HPLC, PDA, MS, NMR, MP, EA, XRD, XRF, RAMAN…). Acidic activation was important for the preparation of homogeneous catalysts. The procedure were optimized for the preparation of conjugates as heterogeneous carriers for deposition on fabrics, an important step was Soxhlet extraction, to remove unreacted heteroboranes. Than followed the characterization of changes in the physicochemical properties of the newly prepared materials. Esterification was performed in a model mixture of fatty acid using bioethanol.

Research highlights:

1) Some di- and tetrachlorine derivateves of cobalt (bis)dicarbolide anion were used as homogenous catalysts
2) Evidence from XRF that cobalt is presence as a heavy sandwich atom in cluster on the polymer surface
3) Changes in wettability angle of modificated textiles

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Isolation and characterization of plant exosomes for biomedical applications

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Exosomes are small membrane nanoparticles naturally produced by various cell types, including mammalian, fungal and plant cells. For their specific properties, such as the presence of plasma membrane on their surface, size (usually 30 – 150 nm) and the possibility to transfer various molecules, such as small RNAs or proteins, they are able to enter recipient cells and to regulate their physiological processes. Although it was no clear for a long time whether plants release exosomes, today we know that it is so [1–3]. It was shown, plant exosome-like nanovesicles (PELNs) are able to enter cells of different species, including human, where they can modulate physiological processes. PELNs were proven to have therapeutic effects in diseases, such as cancer, inflammatory diseases etc. Due to ideal native structure and properties, exosomes appear to be a suitable drug delivery vehicles, as they are able to encapsulate the drug, cross the plasma membrane and deliver the drug into the target site without eliciting an immune response from the recipient organism [4–7].

This research is supported by three-year student project (SGS UJEP). Our goal was to compare different plant materials for PELNs isolation, including new sources, such as toacco callus and tobacco suspension cultures and to select the most suitable method of exosome isolation. We performed biophysical analysis using Dynamic Light Scattering and Nanoparticle Tracking analysis and biochemical protein analysis. PELNs were labeled using Bodipy TR Ceramide to investigate their ability to enter various cell types.

Research highlights

1) We isolated tobacco-derived exosomes using two methods if isolation, namely ultracentrifugation and polyethylene glycol precipitation.
2) We determined PELNs size, concentration and protein concentration.
3) We confirmed the presence of exosomal marker.
4) We observed the uptake of labelled PELNs by mesenchymal cells and by tobacco cells.

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1D Model of a Heat and Mass Transfer in a Rotary Kiln

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The rotary kiln is widely used in the civil, metallurgical and chemical industries especially for drying, reaction, mixing, granulation and heating of granular materials. For the above reasons, it is essential to investigate heat transfer phenomena in order to improve modeling tools and understand the dynamics of heat and mass transfer in rotary kilns.

The rotary kiln under study is a low-angle cylinder 0.5 m long and 0.108 m in diameter with regularly arranged lifters on the inside and hot air on the inlet. The number of lifters in the rotary kiln ranged from one to twenty-five. The load in the rotary kiln consists of spherical particles with a diameter of 1 millimeter. The volume fraction of the load is 15 %. The rotary kiln rotates at 21.5 rpm. For each simulation, 20 rotations were performed. The discrete element method (DEM) implemented in the open-source code LIGGGHTS was used for the simulations. Furthermore, simulations were performed for the same geometry and physical conditions using a 1D model of heat and solid phase transport in a rotary kiln in order to calculate the volume fraction of the so-called active phase, i.e., the particles in the updraft that contribute most to heat transport in the kiln. Additional data processing was performed in Matlab and Paraview.

By comparing and interpreting the results of both methods, it was found that the 1D axial model provides relevant results in the range of one to fifteen lifters. There is also an optimum for fifteen lifters which provides the largest active phase. Also significant was the finding that a larger number of jacks than this optimum does not contribute to an increase in the active phase. However, the 1D axial model also provides an increase in the active phase for a larger number of jacks, which is contrary to the physical reality observed by the discrete particle model visualization.

Research highlights

1) The range of lifts at which the 1D model provides relevant results was determined.
2) The active phase controlling the optimal heat transport is highest for a number of lifters around fifteen.

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This research was supported by the project U21-Kvalitní lidské zdroje pro posílení mezinárodního prostředí II CZ.02.2.69/0.0/0.0/18_053/0017815 and by the internal grant UJEP-SGS-2020-53-003-3.

Molecular simulation of salt hydrates

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Salts are among the most important substances on the Earth. Molecular simulation studies of salts dissolved in aqueous solutions and of their anhydrous crystals have become relatively common, particularly for rock salt (NaCl) and its aqueous solutions. However, almost nothing can be found in the literature regarding molecular simulations of crystalline salt hydrates (e.g., $LiCl \cdot H_2O$, $LiCl \cdot 2H_2O$, $NaBr \cdot H_2O$). The first successful molecular simulations of salt hydrates appeared in the literature only recently and only in the case of hydrohalite ($NaCl \cdot 2H_2O$). Therefore, it is not surprising that neither results of the properties of crystalline hydrates obtained from molecular simulations nor a description of the relevant methodology can be found in the literature.

Our study focuses on the determination of the structural properties of alkali-halide salt hydrates from molecular simulations, including their ability to qualitatively predict experimentally known crystalline structures and quantitatively predict the corresponding crystal lattice parameters. Our Monte Carlo molecular simulations using state-of-the-art polarizable models developed recently in our group [1, 2] show that the models predict crystal lattice structures in agreement with experiments, with lattice parameters that deviate only negligibly from experimental data. Furthermore, we attempt to elucidate the spatial distribution of Li^+ cations in the structure of lithium iodide monohydrate ($LiI \cdot H_2O$), which is described experimentally rather vaguely as stochastic.

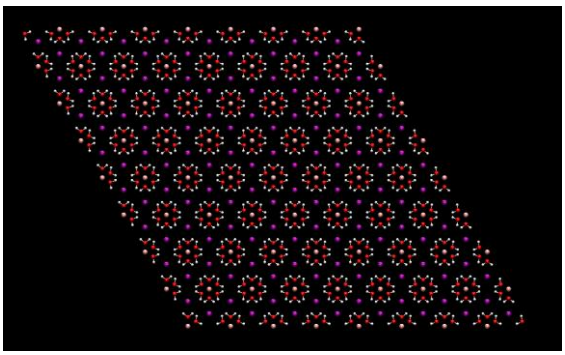

Figure 1: Initial configuration in the molecular simulation of crystalline $LiI \cdot 3H_2O$.

Research highlights
1) Molecular simulations of crystalline hydrates in agreement with experiments.
2) Can molecular simulations elucidate the structure of $LiI \cdot H_2O$?

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Covalent functionalization of MXene flakes for stable and biocompatible MRI contrast agent

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MXenes are an excellent candidate for medical applications, including diagnostic approaches such as positron emission tomography, computed tomography, and magnetic resonance imaging (MRI). However, the utilization of MXenes for bioimaging is restricted by their commonly diamagnetic nature. MXenes can be functionalized using ferromagnetic or paramagnetic compounds and nanoparticles to develop efficient bioimaging tools. In contrast to previously published approaches based on electrostatic interactions, covalent approaches could enhance MXene stability and prevent self-aggregation with degradation. This work proposes covalent functionalization of Ti_3C_2T flakes with a chelating agent diethylenetriaminepentaacetic acid (DTPA) and further complexing with Gd^{3+} ions. The developed functionalization procedure provides a paramagnetic response to the intrinsically diamagnetic Ti_3C_2T flakes for T1-MR imaging. Moreover, we observed the apparent dependency of magnetic relaxation time on the flake concentration, which enabled us to estimate the spatially resolved flake distribution. The covalent decoration strategy for MXene led to surface protection against oxidation in phosphate buffer saline and blood serum, accompanied by increased cytocompatibility. Moreover, chelation of Gd^{3+} ions prevented leaking compared with electrostatic chemisorption. We demonstrated a high degree of photothermal conversion efficiency of MXene-Gd, anticipating future application in photothermal therapy. This work broadens the bioapplication of MXenes, not only by introducing an MRI contrast but also by developing covalent functionalization strategies for MXenes.

Research highlights

1) The covalent functionalization of MXene with diethylenetriaminepentaacetic acid was proposed.
2) MXene-DTPA complexing with Gd^{3+} provided paramagnetic response to the diamagnetic MXene.
3) MXene-Gd showed oxidative resistance in phosphate buffer saline and blood serum.
4) The chelation of Gd^{3+} ions by MXene-DTPA prevented leaking to bioliquids.

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Fuel characteristics of *Miscanthus x giganteus* biomass produced at the marginal and slightly contaminated by trace elements soils

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Miscanthus x gianteus has been identified to be successful in the remediation of slightly contaminated sites by TEs or marginal lands with production of biomass for bioproducts or energy [1]. The use of *M.xgiganteus* biomass as an alternative energy source positively contributes to climate change mitigation. The aim of this study was to analyze the properties of *Mxg* biomass in thermochemical transformation by gasification and how the process may be impacted by conditions of the background production of the crop. Varied combustion properties of *Mxg* from different locations and plantation types were investigated. The input materials from two plantations in Ukraine (marginal-Tokarivka) and contaminated (NULES, Kyiv), Croatia (agricultural), and Czech Republic (post military-Chomutov) were evaluated. Biomass from all locations were analyzed as a mixture of leaves and stems, in addition, leaves and stems were analyzed separately for biomass from Croatia and Kyiv. The proximate analysis (determination of ash content, total water, volatile matter, and fixed carbon), calorific value, and ultimate analysis (content of C, H, N, and S) were done based on German and international standards (DIN and DIN ISO). The ash melting behavior of samples was analyzed using heating microscope with software EMI III as criteria for the material´s applicability in biomass gasification: a low ash melting temperature can lead to slagging of the process and thus to serious technical problems during gasification [2]. In accordance to the literature data [3] final melting for low meltable ashes is from 1000 to 1200 °C, for medium meltable ashes is from 1200 to 1450 °C, and for heavy meltable ashes is over 1450 °C.

Results showed that ash content and volatile matter of the various *Mxg* are significantly different based on the location and ranging in average 4.9% and 78.1% , respectively. The calorific value of the the biomass from different locations was high for all tested samples, ranging from 18 to 19 MJ/Kg. The highest calorific value was received for *Mxg* produced in Kyiv despite Pb contamination in soil. The average final melting temperature of the mixture of *Mxg* leaves and stems was 1323 °C, a medium meltable ash, suitable for gasification. The next step in the research will be commercial gasification of the *Mxg* biomass in order to receive residual "ash" to be converted to suitable sorbents.

Research highlights

1) There are differences in properties of *Mxg* produced in different locations.
2) Mixed above ground *Mxg* biomass is suitable for gasification.
3) *Mxg* biomass produced at the marginal/contaminated lands can be gasified successfully.

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All-in-one OSTE+ droplet microfluidic tumor spheroid chip

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We are developing a lab-on-chip microfluidic system capable of forming tumor spheroids from cell suspension in individual generated water droplets in oil, coalesce the droplets back into one water phase inside the system once the spheroids are formed, transfer the released spheroids into cultivation part with trapping elements and cultivate them long-term in flow-through conditions. This will allow the testing of potential anti-cancer pharmaceuticals on 3D cell cultures, which have much better similarity to real tumors in terms of drug resistance than standard 2D cultures. No hydrogel encapsulation or external handling of the spheroids and droplets is required, everything is done inside one microfluidic chip. The chip is manufactured from OSTE+ (off-stoichiometry thiol-ene epoxy) polymer, by double casting from DLP (digital light processing) 3D printed master, with a PDMS (polydimethylsiloxane) intermediate negative master. The chip is repeatedly useable, as the fully cured OSTE+ polymer can be effectively cleaned by sonication in isopropanol, ethanol and water.

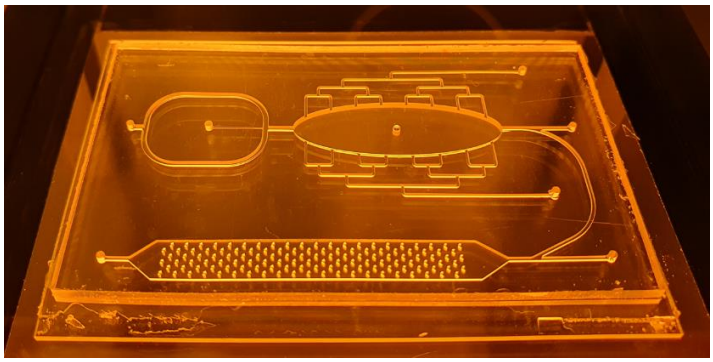

Figure 1 Current version of our microfluidic chip made from OSTE+ after first UV cure. The chip contains droplet generator, reservoir for the generated droplets, side branches for flushing with 1H,1H,2H,2H-Perfluoro-1-octanol to coalesce the droplets and an early version of cultivation system with trapping elements for the released spheroids (still in development).

Research highlights

1) OSTE+ polymer was proven to be suitable for manufacturing of repeatedly useable cell cultivation system.
2) A new microfluidic chip for forming and cultivation of tumor spheroids without external handling has been developed.

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Particle Transport in Microfluidic Devices: A Multiscale Modeling Approach

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This work presents a methodology for particle transport in microfluidic devices via multiscale modeling approach. The focus of this contribution was on biotechnological applications and chosen dimensions for performed simulations were in correspondence with particle diameter of biological particles such as fish embryos (mm), cells (μm) and exosomes (nm). In dependence on the ratio of particle size to the microfluidic device dimensions, an appropriate computational technique was used to model two phase systems. Specifically, resolved discrete particle model was used for the case of millimeter particles. For smaller particles, simulations were performed via unresolved discrete particle model. In dependence of interactions between particles and fluid, one-way or four-way coupling was used. In one-way coupling, only fluid affects the particles while particle has no effect on fluid (the case of exosomes). Besides mutual particle-fluid interaction, four-way coupling also assumes particle-particle and particle-wall interaction (cell suspension). Particle trajectory, settling velocity and angular velocity were evaluated for each modeling case. Simulation results were compared to experimental measurements, theory and published data in literature. The obtained results will be used for development and behavior optimalization of new experimental microfluidic devices.

Research highlights

1) Methodology for particle transport via multiscale modeling was proposed.
2) Terminal settling velocity of particles was determined.
3) Conditions of embryo transport in a microfluidic device were presented.
4) Settling velocity is dependent on particle concentration in fluid.
5) Particle separation was presented in dependence of their diameter.

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Acknowledgements: This research was supported from the grant UJEP-SGS-2020-53-003-3 and from Strategy AV21 of the Czech Academy of Sciences, VP20 - Water for life for valuable support.

On-line sensorics and high-resolution mass spectrometry for tropospheric monitoring

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The qualitative composition of the atmosphere has a major impact on the prosperity of the biosphere, yet conventional atmospheric analysis techniques are often limited by sampling frequency and spatial resolution. Recent development of commercially available lightweight gas phase sensors allows to record information about the composition and properties of the atmosphere with high frequency, low energy consumption with small dimensions. These properties make them suitable for development of analytical tools that can be integrated on mobile platforms (multi-rotor or glider drones) to flexibly obtain multiparametric datasets with high spatial resolution. The continuity of the measurement also enables long-term stationary experiments with detection of even short-term deviations of the monitored parameters. However, these sensors usually have several shortcomings that need to be taken into account during interpretation and interpolation of coordinates (response time, noise, limits of quantitation, interferences, …). One of the most environmentally significant factors, in addition to physical parameters and the presence of inorganic gases or aerosoles, is the content of volatile organic compounds in the troposphere. This complex issue is not sufficiently solvable by direct sensorics, therefore it is necessary to take VOC for ex-situ GC-MS analysis, preferably by capture on sorbents. In addition to standard "hard" electron ionization for VOCs analyses, there are also atmospheric ionization techniques coupled to GC-MS that can provide additional or alternative information on the volatile organic compound profile. A deeper understanding of their ionization mechanisms and the building of spectral databases are necessary prerequisites for the maximum number of robust identifications per analysis. In the field of tropospheric sensors, several devices integrating selected sensors have been designed and programmed. Sensors of inorganic gases (electrochemical), volatile organic compounds (photoionization), aerosols (light scattering), temperature and humidity were implemented for mobile analytics from drones. In this asynchronous configuration, several stationary tests and drone installations were performed. Dedicated devices with sensors of this gas were designed for long-term monitoring of ammonia and their long-term stability and performance characteristics were monitored for a better idea of the relevance of the obtained data, while the effect of interferences was evaluated by an alternative technique. In order to expand the possibilities of identification of volatile organic compounds, 3 ionization techniques in combination with GC-qTOF were tested with emphasis on molecular ion yield and the ability to distinguish eg structural isomers and substances with the same molecular weight or homologous series from natural volatile organic compounds and incomplete combustion products.

Research highlights

1) Development of analytical tools and methods for flexible online monitoring af the atmosphere
2) Optimization of the methods and considering uncertanity of inputs
3) Evaluation of ionization techniques for identification of organic compounds

Microfluidic Tissue Barriers

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Blood-tissue barriers, semipermeable single-cell-thick layers of endothelial cells, line all blood vessels and regulate the exchange of substances between a bloodstream and surrounding tissues. As such, they play a crucial role in transport of drugs and therefore their pharmacological effects.

Mimicking blood-tissue barriers by implementing microfluidic technologies promises drug screening platforms that would provide high-throughput and reproducible screening at a significantly lower cost and without ethical dilemmas.

We currently utilize two approaches to creating artificial, microfluidic (blood-)tissue barriers. In the first approach, a polymeric platform is 3D printed from photosensitive resin E-Shell 300 via stereolithography. Nanofibers combining modified chitosan, gelatine and polyethylene oxide are then electrospun straight onto the platform. Created nanofibrous membrane separates two channels of a chip and acts as a scaffold for the growth of cells introduced after final assembly. In the second approach, we utilize standard lithographic techniques to create a system of microchannels from polydimethylsiloxane (PDMS) and polymers based on off-stoichiometry thiol-ene chemistry (OSTE). Primary channels are interconnected by smaller secondary channels designed to be filled by hydrogel. Proper hydrogel acts as a scaffold and supports cell growth, leading to the creation of a tissue barrier separating individual microfluidic circuits.

Our goal is to create a functional tissue barrier model that will serve as an easily accessible *in vitro* drug screening tool.

Research highlights

1) We designed a device combining 3D printing with nanofibrous membrane.
2) We designed a device utilizing microchannels partially filled by hydrogel.
3) We successfully fabricated prototypes based on both approaches.

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Prostat, Glioblastoma and Mammary carcinoma cells derived exosomes: Their isolation, characterization and loading with doxorubicin

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Exosomes (EXs) derived from the plasmatic membranes of cells are important indicators of physiological and pathological processes of the organism as well as individual tissues and cells. EXs can occur in various of body fluids and are significant for transport of informatory and regulatory molecules such as protein, lipids microRNAs or they can function as vectors in pathogenesis. Because of that EXs are considered an additional mechanism for intercellular communication and can fundamentally influence the development of metastases in cancer or the progression of degenerative changes, modulation of immune responses. At the same time, EXs are widely studied for their ability to transport embedded regulatory molecules or drugs and can be considered as an alternative to traditional nanoparticle approaches in drug delivery systems. EXs can cross the blood-brain barrier and are therefore interesting transporters for central nervous system (CNS) therapies. The production and composition of EXs depending on therapeutic approaches is still a little studied area that can provide essential information about intercellular communication during therapy. An unknown topic is also the modulation of EXs after interaction with nanomaterials, the transfer of nanomaterials through EXs, and also the possibility of transporting EXs with nanomaterials to the CNS across the blood-brain barrier. Given the widespread field of nanomedicine and the possibilities that nanomaterials offer, such as targeted drug delivery, minimizing the side effects of drugs themselves, or optimizing drug circulation in the body, the transport of nanomaterials via EXs is an important experimental goal [1-3].

Research highlights

1) We were able to isolate up to $7x10^{10}$ particles using ultracentrifugation.
2) CD9 and CD81 protein markers were determinated in EXs by Western blotting.
3) By incubation, doxorubicin was loaded into EXs with a 9,155% loading capacity.

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Study of transport properties of PEBAX 1657 and PEBAX 2533 membranes

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The study of the permeability of organic vapours through polymer membranes and their potential applications for the separation of volatile organic vapours is nowadays important due to the ever-increasing demands on air quality [1]. The studied polymer was poly(ether-block-amide): PEBAX 1657 and PEBAX 2533. All the membranes used were prepared at the Department of Chemistry at Jan Evangelista Purkyně University in Ústí nad Labem and at the Institute of Chemical Processes of the Czech Academy of Sciences.

The basic characterization of the used polymers PEBAX 1657 and PEBAX was performed by thickness measurements. This confirmed the homogeneity of the prepared membranes. Furthermore, the potential use of polymer membranes for the separation of volatile organic vapours from air was discussed based on the results of permeation measurements with selected organic substances [2]. Among the selected substances studied - hexane, 2,2,4-trimethylpentane, cyclohexane and ethanol - the highest organic vapour trapping was observed in the case of hexane.

Research highlights:

1) High percentage removal of volatile organic compounds was observed in PDMS membrane.
2) High selectivity for VOCs was found for the PEBA 2533 membrane.
3) The most suitable ionic liquid for the preparation of IL-polymer membranes was butyltrimethylammonium bis(trifluoromethylsulfonyl)imide.

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Shale gas and carbon dioxide adsorption and diffusion in dual-porosity kerogens from molecular simulations

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Computer Methods in Science and Technology

In today's world of rising energy demands, there is strong push for alternative energy resources – and one of those is shale gas. The shale gas, predominantly consisting of methane, ethane, and propane, is stored in shale, consisting of organic and inorganic parts. Most predominant component of shale's organic part is kerogen – which is basically unfinished oil. The shale gas is extracted by hydraulic fracturing and the extraction can be enhanced by carbon dioxide. Shale also shows affinity for the carbon dioxide and thus can be useful for its sequestration.

We use microporous 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. Those models (with added cylindrical pore of two diameters to encompass dual porosity) are complemented by neutral united models for short alkanes and all atom model with partial charges.

In this work, we study adsorption and transport properties of gases in porous kerogens. To determine equilibrium adsorbed amounts, we employ Monte Carlo methods and to evaluate self-diffusion, we use molecular dynamics method. After evaluating chemical potential via constant temperature-constant pressure Monte Carlo method we use inputting chemical potentials in grand canonical Monte Carlo simulation to determine adsorption isotherms at two temperatures. Using the adsorbed amount of molecules as starting point for equilibrium molecular dynamics simulation we use the mean-squared displacement to obtain self-diffusion coefficients.

Research highlights:

1) Realistic kerogen models were deployed and characterised to study species behaviour in those kerogens.
2) Species adsorption generally rises with pressure and decreases with temperature.
3) Species diffusions anti-correlate with the adsorption behaviour.
4) Kerogens show affinity for carbon dioxide.

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Chemical modification of PAN – based nanofibrous membranes prepared by electrospinning and their properties for CO_2 capture potential

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PAN-based nanofiber membranes were prepared by a) needleless (wire) = Nanospider™ and b) needle-based electrospinning techniques. These methods differ in the design of the experiment and especially in the form of the electrodes. These differences are further reflected in the structure and morphology, properties of the resulting nanofiber membrane and the dependence of these properties on the parameters that affect electrospinning. Due to the large number of these parameters, process optimization is a necessary part of the work, ie the selection of the most suitable parameters to achieve the desired properties of the nanofiber membrane.

Thanks to the large specific surface, nanofiber membranes have the potential to capture a variety of particles and molecules. Their properties, especially sorption, can be further modified and improved by modification, while the modification was performed in a so-called one-step = by adding a modifier to the spinning solution and amines and MOFs (metal organic frameworks) were used as modifiers for CO_2 molecule capture potential.

Using a variety of techniques, such as scanning electron microscopy, X-ray diffraction, or the BET adsorption isotherm, the ability of nanofiber membranes to capture CO_2 was subsequently characterized, and improvements in these abilities after modification were revealed in most samples.

Research highlights

1) Needle and wire electrostatic spinning differs in the morphology of the membranes.
2) Rather, the one-step modification leads to clogging of the pores and deactivation of the functional substances.
3) Amines (TETA, TEPA) modifications (wire) resulted in a 3-times improvement in sorption capacity.

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[4] PAN based electrospun nanocomposite membranes for CO_2 adsorption (**manuscript**)

Nanostructuring in carbon-based materials and polymer composites by energetic ion beams to improve electrical and sensing properties

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Graphene oxide material used as precursor for graphene synthetization, as well as organic polymers, have found great potential in sensing and electronic applications in recent years. Such materials usually have high mechanical and thermal resistance, large specific surface area and relatively easy control of their modification [1,2]. Modification of these materials can be performed by doping metal particles onto the surface or into the bulk of the material, which most often provides increased electrical conductivity of the originally non-conductive materials [3,4] and can modify their optical and electrochemical activity. In addition, the extremely large specific surface of these materials is able to absorb more analyte molecules and react to them very quickly, e.g. by changing the electrical resistance or electrical capacitance.

Irradiation of these materials with ion beams leads to changes in the chemical and functional properties that are effective for controlled modification due to the selectable energy, mass and type of ions. In graphene oxide is possible to control the ratio of sp^2/sp^3 hybridization, reduction degrees or dielectric properties. Ion fluence above $1x10^{13}$ at/cm^2 causes the overlap threshold of individual ion tracks and carbon clusters grow with π-bonds. These clusters aggregate within the material and form a network of conjugated chemical bonds [5,6]. Above an ion fluence of $5x10^{13}$ at/cm^2, a high increase in nucleation and aggregation of carbon-enriched clusters on the order of nanometer is expected. This process proceeds until the formation of a quasi-continuous carbon buried layer [4]. The implantation of metal particles above the ion fluence of $1x10^{16}$ at/cm^2 can lead to metal nano-particles formation which is adopted as the next sensitivity promoters [3].

The instrumental development has been carried out at the CANAM (Centre of Accelerators and Nuclear Analytical Methods) infrastructure LM 2015056. This publication was supported by OP RDE, MEYS, Czech Republic under the project CANAM OP, CZ.02.1.01/0.0/0.0/16 013/0001812. The scientific results were obtained with the support of the GACR Project No. 22-10536S and the University of J. E. Purkynje project UJEP-SGS-2021-53-005-2.

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Analysis of the effect of CeO_2 nanoparticles on microbial communities in wastewater treatment process

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Common water purification method involves microbial community known as the activated sludge, which plays a crucial role in disposal of toxic and pathogenic agents in wastewater. Potential combination of the organic water purification process with CeO_2 nanoparticles treatment may result in significant change of the whole microorganic biomass. Using material (including inflow wastewater, outflow purified water and an activated sludge) acquired from local wastewater treatment plant a cultivation experiment was established to determine nature of the interaction between CeO_2 nanoparticles and the complex microbial community. To detect loss/growth of the biomass during the cultivation we used spectroscopic methods. Absorbance of each sample has been measured throughout the cultivation. Molecular analysis of the cultivated microbial communities was carried out by an extraction of DNA of each sample, PCR focusing on procaryotic, eucaryotic and fungi organisms, MID/Tag marking to differentiate each sample and next-generation DNA sequencing using platform MiSeq-Illumina. Results comprise data of the sensitivity of thousands of microbial taxa. Our results show a possible outcome of CeO_2 nanoparticles usage in water purification process from a microbiological perspective as well as a possible impacts on microbial communities commonly present in an environment of outflow water from wastewater treatment plants.

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Gypsum technology of separation Li_2CO_3 from Zinnwaldite mineral

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The Czech Republic has significant lithium reserves in the form of mica in the mineral Zinnwaldite. The total reserves of ores with increased lithium content at Cínovec were estimated to have at least 300 Mt with an average metal content of 0.117% Li. [1]

Several technologies of separation Li_2CO_3 from Zinnwaldite concentrate processing have been developed at the Research Institute of Inorganic Chemistry in Ústí nad Labem in the years 1953 to 1967. The gypsum method based on thermal sintering of the concentrate with a $CaSO_4$ and $Ca(OH)_2$ showed the best yield of Li_2CO_3. However, all technology tests in the past were done using alkaline additives of laboratory purity only.

The aim of the research is to modify the original laboratory gypsum method for the use of real additives - technical calcium hydroxide and natural gypsum or energy gypsum. Today, only one mine for natural gypsum is active in Kobeřice near Opava in the Czech Republic. This represents a long transport distance of the raw material of 450 km. Therefore, it would be appropriate to replace natural gypsum from alternative sources. Because Zinnwaldite deposits are located in Northern Bohemia, where themost coal-fired power plants in the Czech Republic are located it's our best option to try to 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 cheaply as certified raw material.

In presented work, we compared the chemical composition of energy gypsum samples from five different coal-fired power plants and two natural gypsum samples from the Czech Republic and Poland. As the most suitable product was energy gypsum from power plant Ledvice and natural gypsum from Kobeřice. These materials have been used as an alkaline additive in the melting.

The melting batch consists of Zinnwaldite concentrate, gypsum ($CaSO_4 . 2H_2O$), and $Ca(OH)_2$ in a weight ratio of 6 : 4,2 : 2. Three melting barches were prepared: a) additives of laboratory purity, b) natural gypsum additives, c) energy gypsum additives. All these mixtures are going to be simultaneously melting at temperatures of 850-1000°C and furnace dwell times of 15-90 minutes. The resulting clinkers are ground, dissolved and leached in water. Each mixture's ideal temperature and melting time willbe compared according to the amount of lithium converted into solution.The composition of the obtained sulphate extracts allows their simple and effective purification. Using K_2CO_3 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) Gypsum technology of separation Li_2CO_3 from Zinnwaldite mineral
2) Utilization of Zinnwaldite Wastes for Recovery of Lithium
3) 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 material with many applications, it is important heterogeneous catalysts [1]. CeO_2 nanoparticles can be prepared by various procedures. Modern green chemistry favours low-temperature one-pot syntheses, especially for potential industrial production. Several processes for the preparation of active forms of cerium oxide have been developed at our workplaces. Some of these forms have the ability to decompose highly toxic compounds such as organophosphorus pesticides [2] or even structurally similar neural paralytic chemical warfare agents such as sarine, soman or VX [3].

Synthesis at low temperature was used in this work [4]. Samples have been characterized by physico-chemical methods such as XRD, XPS, DTA, BET, HRTEM and its degradation activity against parathionmethyl was measured by HPLC-DAD. This contribution is focused on interactions of nanoceria with environmentally important pollutant that can be decomposed or at least sorbed on its surface depending on the solvent. These substances are usually used as pesticides or medicines. A significant motivation is to help to look for ways to reduce the total amount of hazardous substances in the environment. For example, in the group of triazine pesticides, the interactions with the cerium oxide surface change significantly with a small change in structure.

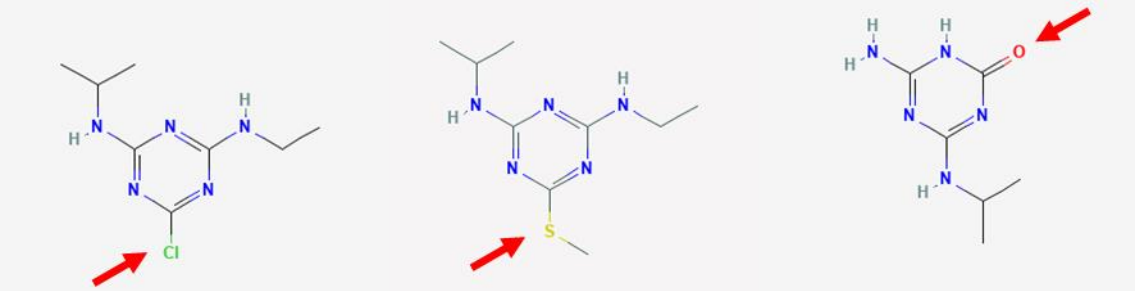

Figure 1 Triazine pesticide from left Atrazine, Ametryn and Atrazine-desethyl-2-hydroxy

Research highlights

1) Optimized synthesis of CeO_2 nanoparticles under ambient conditions in water
2) Large differences in the interactions of structurally similar substances
3) Influence of solvent on the interaction of pollutants with CeO_2

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Expression of multiple galectins in glioblastoma cell lines and exosomes

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Galectins represent a family of lectins, which are glycan-binding proteins that play a crucial role in oncogenic processes. They are involved in tumor cell proliferation, differentiation, migration and oncogenic signalling [1]. Especially, in glioblastoma - the most agresive tumour of CNS, galectins are significantly involved in processes as angiogenesis, chemo-/ radioresistance, cell migration and modulation cell death pathways [2].

Here we report a characterization of the expression of galectin - 1, 3, 8 and 9 in human glioblastoma cells, cultivated in 2D or 3D conditions - spheroids and exosomes derived from U87 and GaMG cell lines. The exosomes from 2D cultures and spheroids were collected by ultracentrifugation and then characterized by BCA assay (concentration of protein) and DLS (size and homogenity). To characterize galectins expression, western blotting was performed.

Through DLS, the radius of the exosomes derived from GaMG and U87 cell lines ranged between 50-350 nm and 50-290 nm. Gal-1, 3 were detected in the both (GaMG and U87) cell lines, cultures (2D and 3D) and even in the exosomes derived from these models. Gal-8 were also found in both cell lines, but not in the 3D cultures and exosomes. Only the Gal-9 has not yet been found in any of the systems studied.

In the next phase of our research, we want to focus on the study of new glycodendrimers/polymers targeting gal-1, 3 or 9. These nanoparticles would be tasked with binding the galectins on the cell surface and thus affect cell migration.

Research highlights

1) Through BCA and DLS, we characterized the exosomes of two cell lines and two cell models

2) We have detected or disproved the presence of four galectins in 2D, 3D cultures and exosomes derived from these cell cultures

3) We want to study the influence of glycodendrimers on the expression of galectins

References

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