Topics of dissertation thesis

Study program: P0712D130003 – CHEMICAL AND ENVIRONMENTAL ENGINEERING
Study program: P0713D070002 – THERMAL ENGINEERING AND FUELS IN INDUSTRY
Study program: P0715D270007 – METALLURGICAL TECHNOLOGY
Study program: P0719D270003 – NANOTECHNOLOGY
Study program: P0788D270004 – MATERIAL SCIENCE AND ENGINEERING

Study program: P0712D130003 - CHEMICAL AND ENVIRONMENTAL ENGINEERING

No.	Supervisor	Title of dissertation thesis	Annotation
1	Ing. Lenka Matějová, Ph.D.	Novel catalysts for catalytic oxidation of volatile organic compounds	The doctoral thesis will bring a knowledge on the preparation and micro/structure of new types of perovskite-based catalysts for the catalytic oxidation of volatile organic compounds (VOCs), especially chlorinated VOCs, which are widely used as synthesis solvents for the production of pharmaceuticals and, thus, represent large-volume toxic waste. Catalytic oxidation (catalytic combustion) is a suitable technology for the reduction of higher concentrations of such VOCs in waste gases. The work will be focused on optimization of the composition of the catalyst in order to achieve its highest possible catalytic efficiency in terms of activity, selectivity as well as stability. It is expected to study the catalytic oxidation of individual VOCs (dichloromethane, perchloroethylene, methanol) and also their mixtures. Attention will also be paid to the description of the mechanism of VOC oxidation on the new type of catalyst being developed.
2	Ing. Lenka Matějová, Ph.D.	Transformation of various solid wastes to carbon adsorbents by using microwave pyrolysis and their study in air depollution	The doctoral work will bring new knowledge about preparation of carbon adsorbents by using microwave pyrolysis and co-pyrolysis of various solid wastes such as agricultural or animal biomass and polymer waste. The influence of process parameters of microwave pyrolysis and the composition of initial feedstock on the mass balance of the process and quality of products (pyrolytic gas, oil and char) will be investigated. In order to utilize carbon/char as an adsorbent for vapours of volatile organic compounds from a waste gas the micro/structure, texture and surface functionalization of carbon will be examined in dependence on the waste composition and used activation by using proper instrumental methods (e.g. physisorption, SAXS, XPS, TEM, Raman spectroscopy, FTIR etc. In the frame of the work the sorption performance of prepared carbon adsorbents for vapours of volatile organic compounds (xylene, methanol etc.) will be verified and will be correlated with carbon physico-chemical properties. The output of the doctoral work should be the revelation of the proper microwave pyrolysis conditions (including possible activation) and the feedstock composition leading to the most efficient carbon adsorbent for selected VOC and the definition of realistic advantages and disadvantages of microwave pyrolysis compared to conventional one.

Study program: P0713D070002 - THERMAL ENGINEERING AND FUELS IN INDUSTRY

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Vlastimil Matějka, Ph.D.	Functionalization of 3D printed ceramic surfaces	Within the frame of dissertation thesis, the possibility of using 3D printing to print ceramic materials will be studied. The surface of 3D printed samples will be further modified to achieve self-cleaning capabilities. The modification of the surfaces with photocatalytically active materials will be used to achieve self-cleaning properties. The prepared photocatalytically active materials will be based on graphitic carbon nitride and its composites with titanium dioxide. The prepared materials will be characterized by selected methods of chemical and phase analysis, methods of electron microscopy, self-cleaning capabilities of the modified 3D printed ceramic surfaces will be tested by discoloration of rhodamine B applied on the surface of prepared samples.

Study program: P0715D270007 - METALLURGICAL TECHNOLOGY

No.	Supervisor	Title of dissertation thesis	Annotation
1	doc. Ing. Silvie Brožová, Ph.D.	Recovering secondary raw materials from recycled batteries	The issue of recycling and circular economy is very topical at the moment. The thesis will deal with the processing of waste batteries and the recovery of selected metals as secondary raw materials for further use in industry. The experimental work of this topic will be directed towards the recovery of a group of light metals from waste batteries. Within the framework of the thesis, the student will obtain the latest information in the field of technological possibilities of processing waste batteries by hydrometallurgical methods. On the basis of the knowledge gained, the technological process, composition, quantity and method of leaching application will be proposed to achieve the desired properties of the metal obtained.
2	doc. Ing. Pavlína Pustějovská, Ph.D.	Study of the possibility of testing fine-grained iron-bearing materials	The doctoral thesis will focus on the study of the possibility of testing fine-grained iron-bearing materials and waste. Design of a method and sampling of selected iron-bearing materials and waste. Gain new knowledge by testing prepared samples. Interpretation of the experimentally determined reduction characteristics for real operating conditions. Application of a kinetic model to predict the course of a blast furnace process using manufactured samples. The goal will be to verify the procedures associated with the appropriate treatment of fine-grained iron-bearing waste materials that could be used as part of the charge in metallurgical aggregates.
3	doc. Ing. Lenka Kunčická, Ph.D.	Study of alternative methods of preparation of Cu-C composite materials	1. Composite materials, introduction. 2. Copper-based alloys and composites. 3. Carbon elements for composite materials. 4. Copper-carbon composites, state of the art. 5. Aims of the work. 6. Design and characterization of experimental works. 7. Evaluation of examined characteristics. 8. Discussion and conclusions. 9. Prospective effects of acquired results in commercial practice
4	prof. Ing. Radim Kocich, Ph.D.	Analysis of the influence of intensive plastic deformation on structure and properties of selected bio-applicable alloys	Titanium alloys are at present preferred in medicine especially due to their favourable properties. They have a wide range of application, from dentistry to orthopaedics. Nevertheless, each type of application demands slightly different properties of the given product, which goes hand in hand with variations in structure. The dissertation work will be focused on characterization of selected titanium or magnesium based alloys subjected to the influence of intensive plastic deformation. Plastic deformation will be imparted into the processed materials via conventional, as well as unconventional forming technologies. The emphasis of the work will be on the analysis of mechanical properties and structure changes related to the particular applied deformation technology. Besides, verification of the influence of deformation ratio and the method of imposing the strain into the material on deformation parameters is planned to be performed.

5	prof. Ing. Radim Kocich, Ph.D.	The study of possibillities for composites production by technologies based on plastic deformation	Thesis should be focused on theoretical as well as experimental evaluation of composite materials preparation. Each production technology will be evaluated in view of structure as well as properties changes of composites. Among others computer simulations will be used in order to predict material behaviour. Obtained values will be compared with the results arisen from numerical predictions.
6	prof. Ing. Radim Kocich, Ph.D.	The possibilities of forming methods application in ODS materials with higher properties and thermal resistance manufacturing	The aim of this thesis would be in the study of effectiveness of chosen forming processes in view of their suitability for compact bulk materials. Besides, interest will be paid on the grain refinement effectivity or more precisely on final properties. Among others, conventional as well as unconventional forming methods will be studied. Main attention would be paid on monitoring of mechanical properties in particular under higher temperatures. The focus will be devoted also to the possibility to spread these manufacturing methods into commercial scale.

Study program: P0719D270003 – NANOTECHNOLOGY

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Kamila Kočí, Ph.D.	CO_2 transformation to valuable chemicals by photocatalytic processes over highly active materials	The main goal of the work is to describe the fundamental facet of the effects on the activity of prepared materials in the CO_2 transformation and to clarify the relationship between the activity, selectivity and stability of materials and their physico-chemical properties.
2	Ing. Dominik Legut, Ph.D.	Heat transfer in advanced nuclear fuels	The uranium, plutonium, and thorium carbides as well as the mixed uranium-plutonium carbides are currently being widely studied for their potential application as fuel for propulsion systems and advanced nuclear fuels in the so-called generation-IV reactors with high operating temperature (to maximize efficiency). The advantage over the uranium/plutonium oxides is in higher thermal conductivity and much shorter time of radiating burned fuel to store before getting to radiation background levels (20-30 years). The goal of this Ph.D. thesis is to understand and determine the rules of Nature how to maximize the transfer of the energy (thermal conductivity) by means of quantum-mechanical and molecular dynamical calculations at the IT4Innovations on HPC clusters. More info at www.md-esg.eu.
3	Ing. Dominik Legut, Ph.D.	Modelling of THz laser sources	The energy conversion of between various vibration modes are govern by their coupling and the relaxation time of these modes (their mutual scattering). In this PhD work, based on the quantum mechanical simulations of the anharmonic vibrational effects we will shed a light to the principles how to enhance selected vibration modes to generate THz radiation in solids. For this purpose we will utilize the HPC clusters at IT4Innovations with the state of the art codes for anharmonicity treatment and post-processing. More info at www.md-esg.eu
4	Ing. Dominik Legut, Ph.D.	Design of novel materials for thermonuclear reactors	The purpose of this work is to design novel materials for the plasma-to-coolant heat transfer in the thermonuclear fusion reactors. The expected outcome is a set of experimentally confirmed alloys (together with our team at the Institute of Plasma Physics of the Czech Academy of Science in Prague) able to withstand a critical malfunction (Loss-of-coolant Accident) - the conditions comparable to the ones in Sun's core. The student will perform the calculations on the state-of-the-art HPC clusters located at the IT4Innovation National Supercomputing Center. More info at www.md-esg.eu

5	Ing. Dominik Legut, Ph.D.	Multiscale modeling of coupling phenomena in magnetic material	The objective of this PhD project is to apply advanced modeling approaches and associated numerical tools for a complete fundamental understanding of coupling phenomena in magnetic materials across length scales using HPC clusters located at the IT4Innovation National Supercomputing Center. The project deals with the design of novel permanent magnets with less content or none of the critical and expensive rare earth elements like Nd or Sm. More info at www.md-esg.eu
6	Ing. Dominik Legut, Ph.D.	Modeling thermodynamic properties of liquid-solid interface	The aim of the PhD research is to study the thermal and transport properties of molten salts in the next generation thermonuclear reactors by means of numerical simulations. At the atomistic level, the intrinsic physical properties of crystalline phases of LiF-BeF2 systems will be investigated with ab-initio quantum mechanical calculations. At the nanoscale level, the thermal and transport properties will be studied by large-scale molecular dynamics simulations of the solid-liquid interface between crystalline and molten fluoride salts. The projects aims in general to determined the eutectic point of two phases and be able to model purely from calculations properties of matter close to melting temperatures. More info at www.md-esg.eu
7	prof. Ing. Lucie Obalová, Ph.D.	Preparation of heterogeneous catalysts based on transition metal oxides and lanthanides enriched with active species for catalytic oxidation of volatile organic compounds	The doctoral work will bring new knowledge about the effect of preparation and chemical composition of heterogeneous supported catalyst on its physico-chemical properties (micro/structure, acidity, reducibility etc.) and catalytic activity in oxidation of volatile organic compounds (VOCs) often used as solvents in pharmaceutical industry. In the frame of the work the catalyst preparation and chemical composition will be optimized in order to achieve catalyst highest performance from the view of catalytic activity as well as selectivity and durability. The attention will be also dedicated to the description of oxidation mechanism of selected VOCs on the developed heterogeneous catalyst. Within the catalytic experiments the oxidation of dichloromethane, formaldehyde or toluene will be investigated. Student will partially do the experimental work in cooperation with foreign university via the short-term student stays.
8	doc. Dr. Mgr. Kamil Postava	Mueller matrix polarimetry and microscopy of Twisted light	Nowdays, the progress in wavefront modification have enabled complex classes of Twisted Light which carry spin and orbital angular momentum, offering new tools for light-matter interaction, imaging, detection, communication, and security holograms applications. Spin angular momentum (SAM) arises when the electric field vector traces a helical path with propagation, and takes the values of $\pm\hbar$ per photon, depending on the polarization handedness (i.e., right- or left-hand circular polarization). Orbital angular momentum (OAM) is the phenomena, where the wavefront carries a phase singularity. This is typically realized when the wavefront has helical form producing a one-dimensional (1D) phase singularity – a line of undefined phase (and zero intensity) along the optical path. In this

			case, the Poynting vector precesses around the phase singularity and producing a donut-like intensity profile, also known as an optical vortex. The proposed Ph.D. thesis is focused on study of metasurface structures for generation of OAM Twisted light. For the numerical modelling, the CST Microwave studio (or COMSOL multipsysics) will be used. The modeled structure will be developed by UV laser direct write optical litography. Methods of Mueller matrix spectroscopy and polarimetric microscopy will be used for optical characterization of the fabricated OEM structures.
9	doc. Dr. Mgr. Kamil Postava	Ultrafast properties of spin lasers with periodic gratings: Novel concepts in data transfer technology	Spin-lasers are semiconductor devices in which recombinations of spin-polarized electrons in active region (quantum wells and dots) lead to emission of circularly-polarized photons. The possibility of using and modulate spin-polarized electrons together with including low-dimensional nanostructures (periodical gratings, quantum wells, quantum dots) opens new horizons in modern semiconductor research and information technology. Proposed doctoral thesis will be focused on theoretical and experimental study of steady-state and dynamical effects in such advanced structures together with their optimalization for ultrafast modulation, terahertz generation and secure data transfer. Theoretical models for generation of light from the structures of spin-lasers and thin-film lasers with lateral periodic and aperiodic structures will be applied and generalized. Designed structures will be prepared using technologies at VSB-TUO and foreign collaborating laboratories and their polarization, spectral, and dynamic response will be measured.
10	doc. Dr. Mgr. Kamil Postava	Properties of ultrafast spin-orbit current in magnetic multilayers	Dynamics of spintronic and spin-transport phenomena will be studied using pump-probe technique based on ultrashort pulsed laser beam. The pumped electric pulse will be obtained using Auston switch. Probe beam delayed by optical delay line will inspect magnetic state using magneto-optical effects. Testing structure will be prepared using advance lithography.
11	doc. Dr. Mgr. Kamil Postava	Optimization and design of metasurface and diffracting surface using artificial intelligence	Metasurfaces and diffracting optical surfaces have a wide potencial in planar imaging optics, polarization devices, metrology, and safety elements. The thesis is focused on parametrizing the structure, calculation of optical response, and structure optimization using genetic algorithms and supercomputer facility.
12	prof. Mark Hermann Rümmeli	Synthesis of novel chemically doped graphene and their application	In this project a hybrid chemical vapor deposition/chemical vapor transport fabrication approach will be implemented for the synthesis of chemically doped graphene with novel elements. For example, Be is predicted to be an exciting doped graphene for electrochemical application, but has yet to be synthesized. The potential of the synthesized doped graphene's in applications will be explored in areas such as gas sensors, CO2 capture and as active electrode material in ion batteries.

13	prof. Mark Hermann Rümmeli	Chemical vapor deposition (CVD) of novel substitutional graphene and advanced characterization	This project explores the use of different precursor phases (liquid, solid, gas) for the fabrication of novel metal dopants in graphene. The systematic evaluation of the growth mechanisms will lead to a comprehensive understanding of the growth mechanisms. The work will also involve training and characterizations by aberration corrected transmission electron microscopy and will involve visits to collaborative institutions for training and measurement.
14	prof. Mark Hermann Rümmeli	In situ synthesis and engineering of novel mono and hetero two dimensional materials	In this project a variety of systems will be explored to drive the synthesis and engineering of two dimensional (2D) materials inside a transmission electron microscope (TEM). This will entail the fabrication and engineering of 2D materials using electron beams and heat as well as gas injection in situ in a TEM using custom build TEM specimen holders/reactors. The studies should lead to deep insight to the processes at the atomic scale.
15	prof. Mark Hermann Rümmeli	Combined Electron Beam and Thermal Processes for Enhanced Nanomaterial Synthesis	This research will investigate the combined use of electron beam technology and thermal processes to synthesize nanomaterials with enhanced properties. The project aims to understand how thermal energy can be integrated with e-beam techniques to influence material growth and structural features at the nanometer scale. The PhD candidate will focus on how these dual techniques can be used to improve material crystallinity and functional properties, providing new insights into the controlled fabrication of complex nanomaterials.
16	prof. Ing. Gražyna Simha Martynková, Ph.D.	Nanometal particles in conductive polymers for energy applications	This work focuses on the issue of incorporation of metal nanoparticles into various types of biopolymer matrices and their copolymers. The resulting composites will take the form of a thin film or fibrous fabric, with a set of nanometals – Ag, Cu, and V – homogeneously dispersed in the matrix. Metal nanoparticles are synthesized in an environmentally friendly way without the use of toxic substances. The composites will be tested for electrical and mechanical properties. The characterization of nanocomposites will be focused on the analysis of surface morphology, distribution of nanoparticles in the matrix and changes in the phase composition of individual components. A detailed study of the interactions between the components of the composite will be complemented by molecular modeling, where the model will be compared with the experiment.
17	prof. Ing. Gražyna Simha Martynková, Ph.D.	Advanced Methods for the Preparation of High-Quality Graphene	Graphene, a single layer of sp^2-hybridized carbon atoms arranged in a hexagonal lattice, has emerged as a material of remarkable scientific interest due to its unique structural and intrinsic properties. This thesis presents a comprehensive study of advanced methods for the preparation of graphene, focusing exclusively on the material itself. Emphasis is placed on both mechanical and chemical exfoliation techniques, chemical vapor deposition (CVD). Each method is analyzed in terms of graphene layer quality, structural integrity, defect formation, and control over thickness and lateral size. The work also considers the influence of process parameters on crystallinity and surface morphology, supported by extensive

			characterization using X-ray diffraction methods (XRD), Raman spectroscopy, atomic force microscopy (AFM), and scanning and transmission electron microscopy (SEM/TEM). By systematically comparing the strengths and limitations of each approach, this study aims to identify optimal strategies for producing graphene suitable for fundamental research and material science advancements.
18	prof. Ing. Gražyna Simha Martynková, Ph.D.	Membrane composites with nanofibers for the batteries	The doctoral thesis is focused on the preparation, study and characterization of membrane nanocomposites for parts of batteries, namely flow-through batteries (Redox-flow batteries (RFB) and parts of Li-batteries (LiB), where the membrane is a separator. Nanocomposite membranes will contain carbon nanoparticles and other suitable layered nanomaterials embedded in the matrix to improve membrane properties. Conventional MIVs are of ionic polymers such as sulfonated tetrafluoroethylene polymers with the drawbacks of relatively low ion selectivity and reduced material stability (co with Prof Ramani, WU, USA). The topic of separators in LiB is period where the development of a selective membrane that would extend the cycling life of rechargeable batteries by preventing the formation of unwanted dendrites (in collaboration with dr Slavík, Theion, Germany) By combining advanced technologies together with nanotechnologies, a membrane with stable chemical and thermal properties for specific batteries ity molecular modeling approaches, where optimal physical and structural parameters will be modeled based on the experiment.
19	prof. Ing. Gražyna Simha Martynková, Ph.D.	Application of nanometal particles in conductive polymers for energy applications	The work is focused on the special topic of incorporating metal nanoparticles into various alternatives of bio-polymer matrices and their copolymers. The composite will be in the form of a thin foil or fiber fabric. A set of nanometals -Ag, Cu and Ti- is homogeneously dispersed in the matrix. Metal nanoparticles are prepared in a bio-sustainable way without toxic substances. The composites will be tested for electrical and mechanical parameters. The characterization of nanocomposites is focused on the morphology of the surface of the composite, dispersion of nanoparticles and changes in the phase composition of individual components. An intensive study of component interactions will be complemented by modeling.
20	prof. Ing. Gražyna Simha Martynková, Ph.D.	Nanoporous carbon for bones scaffolds	The thesis is focused on the study and research of meso and nanoporous carbonaceous material with graphitic structure. The preparation of the material is accomplished by carbonization of the macromolecular precursor material and high temperature treatment in an inert atmosphere. Carbonized material is used as scaffold for dental or small bones, and it is densified with biopolymer such as collagen for better biocompatibility and bioceramic for regeneration. The testing of biostability and structural properties will be one of the main goals. The evaluation of biocarbon materials will be characterized using the following methods: porosimetry, XRD, SEM with AFM, XRFS, ICP.

21	Dr. Monika Kinga Michalska	Development of Advanced Materials for Photocatalytic Hydrogen Production and Storage: Focus on Transition Metal Oxides and Graphitic Carbon Nitride	This research aims to explore the potential of novel materials for efficient photocatalytic hydrogen production and storage, which is critical for sustainable energy solutions. Transition metal oxides (TMOs) are considered promising candidates for photocatalysis due to their unique electronic structures, tunable properties, and photocatalytic stability. Specifically, TMOs such as titanium dioxide and iron oxide have shown significant activity in hydrogen evolution reactions (HER) under solar irradiation. Graphitic carbon nitride (g-C_3N_4) has also garnered attention as a metal-free photocatalyst with excellent photocatalytic performance and stability, making it a viable alternative to TMOs. This study will investigate the synergistic effects of combining TMOs and g-C_3N_4 to enhance the photocatalytic efficiency and stability of hydrogen production systems. Furthermore, the materials will be evaluated for their capacity to store hydrogen through adsorption or other mechanisms, thereby addressing the storage challenges of hydrogen as a clean energy carrier. The thesis will explore novel synthesis methods for creating hybrid materials and optimizing their electronic and structural properties for improved photocatalytic activity. In order to understand the relationship between the materials' structure and catalytic performance, advanced characterisation techniques, such as X-ray diffraction, thermal analysis, electron microscopy, BET, and spectroscopic analysis, will be employed. Finally, the scalability and potential for practical applications of these materials in real-world hydrogen production and storage systems will be assessed, contributing to the development of sustainable energy technologies. This work is expected to contribute to the advancement of our understanding of materials design and innovation in the context of renewable energy solutions.
22	Dr. Monika Kinga Michalska	Engineering of g-C3N4/MOF Heterostructured Photocatalysts for Advanced Photo(electro)chemical Hydrogen Evolution	"This PhD project aims to design and synthesize advanced hybrid materials based on graphitic carbon nitride (g-C3N4) and metal–organic frameworks (MOFs) for efficient photo(electro)chemical hydrogen production. The research is highly timely in light of the recent Nobel Prize in Chemistry, which was awarded for the development of MOFs, highlighting their transformative potential in catalysis and energy-related applications.

Study program: P0788D270004 - MATERIALS SCIENCE AND ENGINEERING

No.	Supervisor	Title of dissertation thesis	Annotation
1	Dr. Monika Kinga Michalska	Transition Metal Oxides and Sulfides Doped by Metallic Nanoparticles for Energy Applications	This PhD project aims to design, synthesize, and systematically investigate zinc- and sodium-doped transition metal oxides (TMOs) and transition metal sulfides (TMSs), their composites with metallic nanoparticles and conductive carbon-based materials, as well as their interfacial interactions with functional electrolytes for advanced energy-related applications. The project addresses current challenges in sustainable energy conversion and storage by focusing on material-electrolyte interfaces and their impact on device performance. Transition metal oxides and sulfides are highly attractive functional materials due to their structural diversity, redox activity, and tunable electronic properties. Controlled doping with Zn2+ and Na+ ions will be employed to modify crystal structure, defect chemistry, charge carrier density, and electrical conductivity. In parallel, the incorporation of metallic nanoparticles (e.g., Ni, Co, Ag) and conductive carbon materials (such as graphene, reduced graphene oxide, or porous carbon) is expected to enhance charge transfer pathways and electrochemically active surface area. In addition to electrode material design, the project will include the development and optimization of high conducting gel, or solid-state polymer electrolytes tailored to the prepared TMO/TMS-based electrodes. Particular attention will be paid to electrolyte composition, ionic conductivity, electrochemical stability window, and compatibility with doped oxide and sulfide surfaces. The influence of electrolyte chemistry on interfacial charge transfer, ion transport, and material degradation mechanisms will be systematically studied. The materials will be synthesized using advanced chemical and physico-chemical routes and comprehensively characterized by X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM/TEM), energy-dispersive spectroscopy (EDS), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and Brunauer-Emmett-Teller (BET) surface area analysis. Electrochemical and electrical properties will be evaluated using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic techniques under relevant operating conditions. The expected outcome of this research is a fundamental understanding of structure-property-interface relationships in doped transition metal oxides and sulfides, their composites, and associated electrolytes. The project aims to contribute to the development of stable, efficient, and scalable material systems for next-generation energy conversion and storage technologies, supporting the transition toward sustainable and low-carbon energy systems.

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