Topics of dissertation thesis

Study program: P0413D270001 – MANAGEMENT OF INDUSTRIAL SYSTEMS
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 – MATERIALS SCIENCE AND ENGINEERING

Study program: P0413D270001 - MANAGEMENT OF INDUSTRIAL SYSTEMS

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Petr Besta, Ph.D.	Increasing the efficiency of industrial technologies	The topic of the doctoral thesis will be focused on the optimization of production technologies. The goal will be increasing production efficiency and reducing negative impacts on the environment.
2	prof. Ing. Petr Besta, Ph.D.	Advanced planning in logistics processes	The topic of the doctoral thesis will be focused on increasing the efficiency of logistics processes. While focusing on manufacturing businesses. The solution will be based on advanced planning principles.
3	doc. Ing. Adam Pawliczek, Ph.D.	Dynamic strategic analyses and adaptable business strategies in the era of digitization and global changes	Creating successful strategies in a rapidly changing environment using big data analytics, predictive modelling technologies and strategic planning tools. The topic will focus on effectively adapting strategies to current challenges such as changes in the global market, climate change and technological innovation so that organizations remain competitive.
4	doc. Ing. Adam Pawliczek, Ph.D.	Modern digital management tools for increasing competitiveness in the era of Industry 4.0 and artificial intelligence	Research on the use of digital platforms, robotics and AI to manage and optimize processes, productivity and efficiency in organizations. Emphasis will be placed on the implementation of tools in the field of process automation, data analysis and decision-making models that enable a faster response to market changes and improve long-term competitiveness.
5	doc. Ing. Šárka Vilamová, Ph.D.	Price dumping of metallurgical products as unfair competition	"Metallurgy is historically a very important industrial area, which has its own specifics, but even in this industrial sector we will not avoid unlawful conduct of competing entrepreneurs, aiming to harm or eliminate competition in the market and thus increase their profits. The aim of the dissertation will be to clarify the issue of unfair competition in the field of metallurgical products with a particular focus on price dumping.

Study program: P0712D130003 - CHEMICAL AND ENVIRONMENTAL ENGINEERING

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Vlastimil Matějka, Ph.D.	Photocatalytically active materials in building industry	The topic of doctoral thesis is focused on the utilization of photocatalytically active materials (photocatalysts) in building industry. Photocatalysts are used in the field of photocatalytic cleaning of water and air and thus contribute to elimination of contaminants in living environment. Application of the photocatalyts in building industry for air purification is promising with respect to the fact that the surfaces of building are in direct contact with surrounding atmosphere. Building materials based on latent hydraulic materials, for example metallurgical slags, represents still not widely used alternative to common building materials based on Portland cement. Application of photocatalytically active materials in the mixtures of latent hydraulic materials, or deposited on their surfaces, could further increase the utility value of the resulting products. The aim of the work is to propose and prepare suitable photocatalysts and verify their applicability and functionality in the mixtures of alkali activated latent hydraulic materials. Part of the work will be also focused on the description of the effect of photocatalyst on hydration processes. As the output of the work the formulation of the mixture including selected: i) latent hydraulic material, ii) alkali activator and iii) selected photocatalyst will be proposed with emphasize to acquire the optimal ratio between photocatalytic performance and mechanical properties. The indication of possible specific application of developed material will be proposed as well.
2	prof. Ing. Lucie Obalová, Ph.D.	Chemical recycling of waste plastics by catalytic pyrolysis over structured catalysts	"Chemical recycling is an important alternative to mechanical processes for the recycling of plastic wastes. It offers the possibility of transforming waste plastics into important chemicals which can be used as feedstocks in chemical and petrochemical industries. Thus, chemical recycling of waste plastics has the potential of contributing to resource conservation as well as to waste minimization. Catalytic pyrolysis is an attractive process for the chemical transformation of waste plastic into useful chemicals. The product selectivity during pyrolysis process can be tuned by choosing the appropriate process parameters, catalytic materials as well as reactor configuration. Structured zeolite composites are interesting catalytic materials for the catalytic pyrolysis of waste plastics. They can combine the textural and catalytic properties of zeolites with the geometry (e.g. geometric specific surface) and material related properties (e.g. thermal conductivity) of structured supports. In this regard, a thin layer of zeolite catalyst on a thermally conductive support (e.g. SiC foam) can not only reduce the diffusion path length and maximize the catalyst utilization but also improve the heat transfer inside the reactor.

			The enhanced mass and heat transfer achieved can further improve the activity and stability of the catalyst. The goal of this thesis includes preparation/characterization of zeolite-foam catalyst, testing/determining the optimal conditions of catalytic pyrolysis for selected waste plastics and finding the correlations between physico-chemical and catalytic properties. Requirements: - Completed master's degree in chemical/process engineering, material science, chemistry - Knowledge of analytical methods such as, TGA, XRD, BET, TPD and GC/GC-MS and previous experience with zeolite synthesis/coating would be advantageous but not required.
3	doc. Ing. Michal Ritz, Ph.D.	Use of Raman spectroscopy and Raman microscopy in the analysis of processes taking place on photoactive surfaces	"Raman spectroscopy is a very important analytical method that is applied not only in many fields of scientific research, but also in a number of industrial laboratories. Its great advantage lies in the simplicity of the measurement, which enables both mobile analysis and, for example, connection with optical microscopy. Both of these above-mentioned analytical approaches can be used in the study of photoactive surfaces. Today, these surfaces are the object of many scientific and industrial studies, which very often deal with the self-cleaning ability of these surfaces. Raman spectroscopy can provide very useful and important information about the course and efficiency of processes taking place on photoactive self-cleaning surfaces. The dissertation will be focused on developing a methodology for using Raman spectroscopy and Raman microscopy to study the behavior of photoactive substances during self-cleaning processes. The creation of the methodology will take place in cooperation with research teams that deal with photoactive surfaces at the university. The result should be a methodology applicable both in research and in practice.

Study program: P0713D070002 - THERMAL ENGINEERING AND FUELS IN INDUSTRY

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Vlastimil Matějka, Ph.D.	The influence of the cooling rate on the amorphous character of metallurgical slags	The main aim of the doctoral thesis is the research focused on the indication of the effect of the cooling rate of molten slags on the formation of the amorphous phase. Blast furnace, steel furnace, and ladle furnace slags will be studied. The chemical composition of the slags will be studied using X-ray fluorescence analysis, and the phase composition will be studied using X-ray diffraction method. The slags will be analysed using the method of simultaneous thermal analysis with the aim of revealing the phase transformations during the heating up to the temperatures of liquidus. Melted slags will be further cooled down with predefined cooling rates and the resulting samples of the slags will be analysed using X-ray diffraction analysis to reveal the effect of the cooling rate on the phase transitions, especially on the content of the amorphous phase. With this approach, the optimum cooling rate, which ensures the amorphous character of given slag will be identified. The chemical composition of the slags, which will not spontaneously form a sufficient amount of the amorphous phase even at the highest cooling rates, will be modified by the addition of selected compounds. To reveal the effect of the modification of the chemical composition of the slags, these modified slags will be subjected again to thermal analysis, followed by X-ray diffraction studies of the resulting products. In a theoretical line, the experiments will be supported with the modelling of the phase transitions with the help of appropriate software, for example ThermoCalc.
2	doc. Ing. Adéla Macháčková, Ph.D.	Thermo-technical parameters of the prototype power unit.	Design, specification and verification of the thermo technical parameters of a prototype power unit in the production of electricity, in relation to its accumulation and consumption in a real installation. The solution will use the practical installation of the prototype unit, which is based on the principle of FESS technology. The solution includes a comprehensive approach to the installation as a system from an energy perspective.
3	prof. Ing. Jana Dobrovská, CSc.	Experimental development of paraffin-based solid fuels for hybrid rocket engines	"Paraffin-based solid fuels represent a promising way for the future of hybrid rocket propulsion. Their higher regression rates, improved combustion characteristics, and potential for reduced environmental impact position them as viable alternatives to traditional fuels. On the other hand, these paraffin-based solid fuels also present significant challenges that must be addressed for effective application in propulsion systems. Paraffin wax often exhibits poor mechanical strength and adhesive properties, which can limit its performance in larger rocket engines. Another significant issue is the combustion stability of paraffin-based fuels. Also, the melting point of paraffin wax can lead to issues with fuel consistency and performance at varying temperatures. One way to solve these disadvantages is to prepare

			blending materials: Mixing paraffin with other materials to enhance mechanical properties and structural integrity.
4	doc. Ing. Hana Ovčačíková, Ph.D.	Silicate materials from industrial waste	The dissertation topic is focused on the current trends in the use of waste/material mixtures for the preparation of ceramic materials, pigments and glazes. Suggest new design of materials, shape etc. of interest for industrial applications. In the first step it is necessary to select suitable waste types. Prepare a range of materials for which it will be necessary to verify the functional properties. Establish their characterisation. Calculate the financial balance of product and approach an industrial partner for the application.
5	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	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.
2	prof. Ing. Radim Kocich, Ph.D.	The study of possibilities 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.
3	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 these 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.
4	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.

5	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

Study program: P0719D270003 – NANOTECHNOLOGY

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Daniela Plachá, Ph.D.	Study of adsorption properties of 2D nanomaterials	As part of the dissertation, the interactions of organic molecules with the surface of 2D nanomaterials will be studied. The surface of these materials spontaneously reacts with molecules present in the environment, which affects their further storage and processing, as their properties are significantly affected, e.g. wettability, adhesion, electrochemical properties and also the adsorption properties themselves. Selected organic substances and 2D materials, their mutual interactions and changes in properties will be studied in the thesis. Experimental results will be compared with theoretical calculations of molecular calculations and simulations.
2	prof. Ing. Daniela Plachá, Ph.D.	Development of polymer membranes for wastewater treatment	The dissertation will focus on the preparation of robust and efficient thin-film polymer and polymer nanocomposite membranes suitable for the separation of substances from the aqueous and gaseous environment in industrial applications. The student will focus on the preparation of polymers and polymer nanocomposites in the form of a thin film, including the selection of suitable polymers and nanofillers, as well as on the study of their physicochemical, structural, and mechanical properties. Selected materials will then be used to separate substances from water. The dissertation will be prepared in cooperation with an industrial partner in the Czech Republic.
3	prof. Ing. Daniela Plachá, Ph.D.	Preparation of polymer nanocomposites with antimicrobial effects	As part of the dissertation, polymeric biocompatible nanocomposites with antimicrobial effects with a wide range of applications will be prepared, eg for the preparation of support scaffolds for cell growth with the possibility of using 3D printing or for other biomedical applications. The use of various nanofillers, optimization of material composition and subsequently physicochemical, structural, mechanical, antimicrobial, and cytotoxic properties of prepared materials will be studied. Based on the identified properties, suitable applications will be designed and tested. The dissertation will be prepared in cooperation with ICTP / CSIC in Madrid.
4	prof. Ing. Daniela Plachá, Ph.D.	Carbon supported single metal atom catalyst for water remediation application	Current water purification methods do not provide complete removal of most pollutants and prevention of the penetration of some toxic substances into the environment. The use of a material based on a single metal atom bound to a carbon structure is an alternative way to improve the removal of substances from waters by overcoming diffusion-limited reactions and promoting interactions with target pollutants, including nano- and microplastics, persistent organic pollutants and heavy metals Development of effective catalysts is key to reduce pollution and ensure sustainable development. Single-atom-on-carbon (CSAC)

			catalysts with the advantages of maximum atom utilization, unique electronic structure, and prominent metal-support interaction bring new opportunities for environmental catalysis.
5	prof. Ing. Daniela Plachá, Ph.D.	Designi and synthesis of the single atom with carbon linked covalent organic framework for biomedical application	Single atom with carbon linked covalent organic frameworks (SA-COFs), as an emerging class of ordered and porous crystal material, are mainly composed of light elements (H, B, C, N and O) via the formation of dynamic covalent bonds, and equipped with various unique properties, such as molecular/atomic-level catalytic centers, large surface area, high loading capacity, and homogeneous structure, excellent biocompatibility, tailorable porosity, high stability and crystallinity, and easy modifiability, facilitating it an admirable candidate for biomedical applications. The SA-COF characterized by atomically dispersed active sites, strikingly show utmost atomic utilization, precisely located metal centers, unique metal-support interactions and identical coordination environments. These advantages of SA-COFs drastically boost the specific activity per metal atom, and thus provide great potential for achieving superior catalytic activity and selectivity to functionally stimulate the activity for the biological applications.
6	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.
7	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.

8	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.
9	doc. Dr. Ing. Michal Lesňák	Application of the SPRi method	The subject of our research will be to design biochips for the SPR (surface plasmon resonance) method to measure low concentrations of proteins in solutions. This measurement method can be advantageously used in biochemistry, medicine, pathogen detection in food or military applications. Our method mainly consists of measuring low concentrations of proteins (large organic molecules) in various solutions. Improving the accuracy and speed of measuring low concentrations of proteins in solutions could have a major impact on the quality of medical care provided in hospitals. After discussion with physicians, we decided to focus on the detection of ovalbumin, human serum albumin (HSA) in urine and Cystatin -C.
10	doc. Dr. Mgr. Kamil Postava	Advanced diffraction optical structures in security holography	The main target of the thesis is to design new diffracting structures for applications in security holography. The structure will exhibit special colour effects, 3-dimensional animation effects, polarization selectivity, and light capture. The sample structure will be prepared using laser lithography and physical vapor deposition.
11	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.
12	doc. Ing. Jonáš Tokarský, Ph.D.	Molecular simulation of adsorption on nanocomposite adsorbents and adsorbents prepared from natural materials	The subject of the dissertation is to compare different strategies for simulating the adsorption of molecules on materials with complex and/or difficult to define structure (natural phyllosilicates intercalated and surface modified with organic substances, core@shell structures, activated carbon, etc.). Adsorption simulations on large and complex models of adsorbent structures (very time consuming) will be compared with adsorption simulations on simplified models in order to achieve comparable results and find the optimal degree of

			simplification. The aim of the dissertation is to find simple and fast simulation strategies providing sufficiently accurate results for given types of adsorbents.
13	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.
14	prof. Ing. Jana Seidlerová, CSc.	Biosynthesis of metal nanoparticles by plant biomass and study of nanoparticles formation	The biological way (bioreduction) is an alternative method for nanoparticles preparation. The main goal of this work will be the preparation of metal or metal oxides nanoparticles by biosynthesis (bioreduction) with plants extracts, identification of phytochemicals and other biomolecules which are participating in the bioreduction process and the clarification of the particular biosynthesis mechanisms.
15	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.
16	prof. Mark Hermann Rümmeli	Electron beam manufacture of doped graphene from electron beams	This project explores the use of different composite polymer/metal-organic films deposited on various substrates and the role of electron beam irradiation with and without heating for its local doped graphitization with precision. Different electron beam conditions and temperatures are to be explored systematically through various characterizations as well as complimentary ex situ synthesis to provide a comprehensive understanding of the underlying graphitization mechanisms.
17	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.
18	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.
19	prof. RNDr. Richard Dvorský, Ph.D.	Preparation of sorption nanostructures with photocatalytic regeneration	Sorbents for water treatment and air cleaning is necessary to replace after saturation and dispose of the exposed material. More economical is application of photocatalysis for permanent regeneration by dissociation of pollutants directly on the sorption surface. Very economic process would be regeneration by Solar illumination. The sorption material suitable for photocatalytic regeneration has been prepared in our laboratory and further research is focused on increasing of sorption capacity based on patented method of controlled sublimation.
20	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.
21	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.

22	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 modelling.
23	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.
24	prof. Ing. Jana Seidlerová, CSc.	Stability study of functional nanocomposites	Due to their structural arrangement, clay minerals can be carriers of specific inorganic and organic compounds that can alter their properties. By anchoring molecules on the surface or by intercalation, specific adsorbents or photocatalysts can be prepared. Such a composite must not only have good adsorption, photocatalytic properties, or both adsorption and photocatalytic properties, but must also be stable in each environment. The aim of this work is to prepare a specific nanocomposite and subsequently to observe and describe its behaviour in the environment, to design and validate a method by which stability could be routinely tested.
25	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.
26	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
27	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
28	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
29	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 detemined the eutectic point of two phases and be able to model purely from calculations properties of matter close to melting temperatures.
30	prof. Mark Hermann Rümmeli	Nanoscale Precision Synthesis with Electron Beam-Only Techniques	This PhD project is dedicated to mastering the use of electron beam (e-beam) technology for the synthesis of functional materials at the nanometer scale approaching atomic precision. The candidate will explore the capabilities of e-beams in precisely controlling material properties through direct writing techniques that operate within the nanometer scale. The project will focus on optimizing e-beam parameters such as energy, dwell time, and scanning strategy to refine deposition processes and achieve high-resolution patterning essential for developing advanced nanostructures.
31	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.
32	prof. Mark Hermann Rümmeli	Layer-by-Layer Fabrication of Nanomaterials Using Electron Beam Techniques	This PhD project will focus on developing a layer-by-layer fabrication method using electron beams to construct complex material structures at the nanometer scale. The research will utilize the precise control offered by e-beams to deposit materials sequentially, creating layered structures with each layer defined in the nanometer range. The candidate will study the properties of interfaces between layers and assess the overall stability and functionality of the resulting multi-layered materials, targeting applications in electronics and advanced coating technologies.
33	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 modelling, where the model will be compared with the experiment.

Study program: P0788D270004 - MATERIALS SCIENCE AND ENGINEERING

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. RNDr. Michal Otyepka, Ph.D.	Development of Advanced Biosensors Using 2D Materials	This PhD research focuses on the development of cutting-edge biosensors utilizing advanced graphene derivatives and 2D materials, synthesized through innovative chemical processes. Biosensors are increasingly critical in fields such as healthcare, environmental monitoring, and food safety, where real-time, precise detection of biological and chemical analytes is essential. The candidate will explore novel functionalization techniques for creating highly sensitive and selective biosensors, with applications in these key areas. Emphasis will be placed on optimizing the interface between biocomponents and transducers, and developing scalable, eco-friendly manufacturing processes for these devices. This project offers an exciting opportunity to contribute to next-generation sensor technologies, addressing the growing demand for portable, reliable, and high-performance biosensors in today's rapidly evolving technological landscape.
2	Ing. Martin Négyesi, Ph.D.	Investigating the constraint effect on fracture behaviour of structural steels	Structural integrity assessment requires the knowledge of fracture behaviour. Generally, fracture properties are evaluated by standardized testing methods using standard size and shape specimens. However, a caution needs to be exercised when transferring data from laboratory condition to real components due to the stress triaxiality effect. The stress triaxiality at the crack tip influences the crack growth substantially, and hence, the whole structural integrity. The main objective of the Ph.D. thesis will be to investigate the effect of the stress triaxiality on the fracture behaviour of structural steels employing various specimen shapes and sizes. The experimental testing will be realized through Charpy impact tests and fracture toughness tests as well as tensile tests. Relationships between microstructural characteristics, such as the grain size or precipitates distribution, and the fracture properties will be searched for. The microstructure will be observed using light optical and scanning electron microscopies. Parameters of micromechanical models, which are based on local approaches to fracture, will be found or refined by conducting finite element analysis (FEA). All necessary equipment for specimens testing is provided in Structural Integrity and Material Design (SIMD) laboratory.
3	Ing. Martin Négyesi, Ph.D.	Establishment of advanced instrumented indentation technique (IIT) for in-situ evaluation of material properties	When a flaw is found in a power plant component by non-destructive inspection, it is a serious problem. However, if the flaw is acceptable by failure analyses, and the plant can continue operation for certain periods of time, it is a big benefit to prepare a repair schedule during operation. As a prerequisite for the failure analyses, material properties of the component are indispensable. However, it is not easy to take specimens from the operating

			components. If there is an advanced technique to obtain material properties without component damage, the technique will be employed worldwide. One of such unique methodologies is Instrumented Indentation Technique (IIT). IIT is a novel experimental technique. The objective of this PhD thesis is to establish a new diagnostic tool based on acquisition technique of material properties by using IIT and other related methodologies, such as tensile tests, conventional hardness test, microstructure observation, etc. Structural integrity and failure analyses at operating temperature are to evaluate by the diagnostic tool. Allowable flaws assessed based on IIT data are to reflect actual conditions of piping systems, pressure vessels and other items. Furthermore, IIT data are to serve to propose rules of flaw evaluation for codes and standards. All necessary apparatuses are provided in the Structural Integrity and Material Design (SIMD) laboratory.
4	prof. Ing. Vlastimil Matějka, Ph.D.	Study of the possibility of carbon dioxide capture by carbonation processes	The dissertation will focus on the study of the possibility of using inorganic binder systems to capture carbon dioxide by processes commonly referred to as carbonation. Mixtures for the production of cement-based and latent hydraulic material samples will be designed and tested. Test specimens will be prepared from such prepared mixtures by hydration or an alkaline activation process. Hardened samples will be characterised for the hydration products and their porosity will be assessed. Mechanical parameters, in particular compressive strength, will also be determined. The prepared samples will be further saturated with CO_2 using an autoclave that allows the control of pressure and temperature during CO2 saturation experiments. The carbon content of the prepared samples will be determined as a marker of the level of CO_2 capture, and the phases formed during carbonation will be identified. The experiments will allow to determine the influence of the composition of the mixtures, but also the influence of the porosity of the prepared samples on the CO2 capture rate, thus allowing to indicate the decarbonization potential of the proposed solution.
5	doc. Ing. Petra Váňová, Ph.D.	Study of the degradation effects of hydrogen in structural materials	The issue of hydrogen embrittlement is still relevant in practice and must also be addressed in connection with the development of hydrogen technologies, transport, and storage of hydrogen. During the development of new advanced technical materials, the chemical composition and technological procedures of their production are modified, and thus the microstructure changes. Hydrogen embrittlement is a very serious problem causing degradation of structural components. Structural components operating in a hydrogen environment can absorb hydrogen, which can cause them to fail prematurely when loads below the normal fracture stress level are applied. Therefore, it is necessary to deal with the effect of hydrogen on the possible degradation of their properties. The aim of the dissertation will be to study the degradation effects of hydrogen in gaseous and liquid environments in relation to the microstructural characteristics of structural materials.

6	prof. RNDr. Radek Zbořil, Ph.D.	Deposition and chemical routes of materials for the effective transformation of solar energy	PhD study will deal with chemical routes and deposition methods for synthesis of various semiconductors (TiO_2, $BiVO_4$, Fe_2O_3), which are applicable in photocatalysis and photoelectrochemistry including the technologies of direct solar splitting of water (pure hydrogen production) or photoreduction of CO_2. The student will receive the expertise in advanced synthesis of layered semiconductors via magnetron sputtering technique and materials characterization with a broad portfolio of characterization techniques (e.g. HRTEM, XPS, XRD, SEM, AFM). The approaches of defect engineering and post-processing chemical insertion of single metal atoms will be applied to enhance the efficiency of solar energy harvesting. The specific attention will be devoted to mechanism of action of new nanomaterials combining experimental approaches and theoretical calculations in collaboration with IT4I.
7	prof. Ing. Bohumír Strnadel, DrSc.	Mechanical behavior of low-carbon building materials	The topic of doctoral study will be development and preparation of low-carbon cementitious material. Preparation technology will guarantee the maximum bending strength keeping content of low-carbon cement, saving energy producing building materials, and reducing emission of carbon dioxide. Carbon-fixed cementitious material, and its carbon-negative concrete, will form flexibly a series of low-carbon building material preparation technology, with different applications. The content of low-carbon cement will be optimized to be the bending strength maximal.
8	prof. RNDr. Michal Otyepka, Ph.D.	Development of new materials for inkjet printing	Inkjet material printing represents a revolutionary, flexible, and cost-effective technology for producing a wide range of devices and their components. This technology finds applications in fields such as printed electronics, biosensors, wearable technologies, and Internet of Things (IoT) devices. However, materials and inks suitable for inkjet printing must meet strict requirements regarding properties such as optimal particle size, rheological parameters, surface tension, stability, and adhesion to various types of substrates. The goal of this PhD project is to develop new functional materials and inks for inkjet printing, with a focus on their application in modern technologies such as electrochemical sensors, wearable electronics, and flexible printed circuits. The PhD student will design and synthesize new materials, optimize their properties for compatibility with printing technologies, and test their functionality in selected applications. Special attention will be given to sustainable and environmentally friendly methods for ink production, ensuring compliance with current environmental standards. This project offers extensive opportunities for collaboration with industrial partners and participation in international projects, enabling practical implementation of the developed technologies and expanding knowledge in the field of material printing and modern technologies.