

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: P0715D130002 – CHEMICAL METALLURGY

Study program: P0715D270007 – METALLURGICAL TECHNOLOGY

Study program: P0719D270003 – NANOTECHNOLOGY

Study program: P0788D270004 – MATERIAL SCIENCE AND ENGINEERING

Study program: P0413D270001 - MANAGEMENT OF INDUSTRIAL SYSTEMS

No.	Supervisor	Title of dissertation thesis	Annotation
1	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.
2	doc. Ing. Adam Pawliczek, Ph.D.	Modern management tools for competitiveness regarding the most recent technologies	The work will focus on mapping modern management tools demonstrably leading to higher efficiency and competitiveness of the company with an emphasis on the use of modern technologies such as artificial intelligence, acquisition and analysis of big data, machine learning and the like.
3	doc. Ing. Adam Pawliczek, Ph.D.	Modern risk management in business applications	The work is focused on a comprehensive analysis of risks related to business in today's globalized world. The analysis will be related to a careful search for risk management tools, and they will also formulate strategies for managing risks as well as solving a crisis situation in a specific company.
4	doc. Ing. Adam Pawliczek, Ph.D.	Innovative forecasting using nontraditional methods	The work will explore innovative qualitative methods of forecasting, including the so-called Delphi method, and will use these methods to prepare a forecast of a specific phenomenon or group of phenomena.
5	doc. Ing. Adam Pawliczek, Ph.D.	Commercial applications of modern materials and technologies	The work will focus on mapping the most promising results of recent material research and evaluate the possibilities of commercial use of modern technical materials. Furthermore, business models for specific applications will be proposed.
6	doc. Ing. Adam Pawliczek, Ph.D.	Successful strategies of the new era based upon analyses and cases	The work will focus on the implementation of complex strategic analyzes for the selected company and the formulation of new strategies to ensure the success of the company in the current changing environment. The work will also focus on mapping successful strategies on the market in the selected segment.
7	prof. Ing. Petr Besta, Ph.D.	Modern Technology of Iron and Steel Production in the Context of Increasing the Economic Efficiency of Processes	Environmental requirements affect all production areas. The topic of the doctoral thesis focuses on advanced technologies of iron and steel production. Both the technological area and the impact on the environment will be examined.

8	prof. Ing. Darja Noskievičová, CSc.	Sustainability of digital transformation	The entire digital transformation is based on at least two pillars on the consumer side: Internet access with a fixed price and infinite energy at a reasonable price. The dissertation will be focused on analysis of limitations of today's trend of digital transformation and smart factories building especially in the light of present energy crisis and possible solutions.
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Study program: P0712D130003 - CHEMICAL AND ENVIRONMENTAL ENGINEERING

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Lucie Obalová, Ph.D.	Catalytic destruction of nitrogen containing pollutants	<p>Nitrogen oxides (N₂O, NO, NO₂) and NH₃ are significant pollutants. Many current technologies for reducing these substances in waste gases are economically demanding or require the presence of a reducing agent (ammonia, urea, hydrocarbons) that can lead to emissions of other pollutants (ammonia slip). It is therefore desirable to develop and test new methods for reducing emissions of these components. The main task will be an experimental study of catalytic degradation of nitrogen oxides without the use of a reducing agent and/or oxidation of NH₃ on catalysts containing selected transition metals and a description of the physical-chemical properties of catalysts by available analytical techniques (chemical analysis, X-ray diffraction, physical nitrogen sorption, temperature-programmed desorption and reduction, etc.). The aim of the thesis will be to assess the effectiveness and stability of the materials studied, to clarify the mechanism of ongoing reactions and the relationships between the properties of catalysts and their activity and selectivity, and to optimize the method of catalyst preparation.</p>
2	prof. Ing. Lucie Obalová, Ph.D.	Application in anaerobic digestion of chemically modified biochar and pyro-oil generated from digestate	<p>In a zero-waste approach coupling anaerobic digestion and pyrolysis requires the transformation of the organic matter contained in the digestion solid effluent via pyrolysis to valuable products. The products consist of a pyro-oil including an enriched-in-organics water phase that can be valorized for biogas generation and a solid material (“biochar”) which can be potentially used in several applications e.g. bioremediation, gas cleaning, soil amelioration or as additive in anaerobic digestion. Biochar deriving from biomass pyrolysis has been reported to have a positive effect on anaerobic methane generation. Biochar produced from the solids of the effluent of anaerobic digestion appeared to have lower efficiency. The research study aims to close the cycle between the two processes by initially valorizing the water-phase of pyrolysis oil in biogas production and secondly find appropriate pathways of pretreatment, mainly chemical, for the digestate-derived char to optimize the catalytic activity in an anaerobic digestion system. Laboratory experiments of pyrolysis of separated digestate solids and experiments of its application to laboratory fermenters will be carried out.</p>

3	prof. Ing. Daniela Plachá, Ph.D.	Preparation of polymer membranes for gas and vapor separation	<p>The dissertation will be focused on the preparation of robust and effective thin-film polymer nanocomposite membranes suitable for the separation of gases and vapors in industrial applications. The prepared membranes will be tested for obtaining and purifying hydrogen and for the separation and regeneration of volatile organic substances and other hydrocarbons. As part of the dissertation, the student will be focused on the preparation of polymer nanocomposites in the form of a thin film, including the selection of suitable polymers and nanofillers, as well as on the study of its physico-chemical, structural and mechanical properties, and subsequently will also test the transport of selected gases. The construction of apparatus for separation processes will also be part of the work.</p>
4	prof. Ing. Petr Praus, Ph.D.	Photocatalytic degradation of microplastics in an aqueous environment	<p>The presence of microplastics in the environment has become a real global problem, especially in aquatic environment, such as coastal and marine areas, rivers and other surface water reservoirs. The so-called primary microplastics can be found in everyday products, such as skin scrubs, toothpastes, paints, etc. Secondary microplastics come from the breakdown of larger macroplastic materials under environmental conditions, including sewage treatment plants. The methods of degradation of waste plastics include thermal, mechanical and chemical degradation, ozonation and photo-oxidative degradation. Regardless of the degradation process, various radicals are generated that break down plastics into end products such as hydroxides, peroxides, ketones, aldehydes, carboxyls and CO₂. This process is usually accompanied by a decrease in molecular weight. The photocatalytic process is based on the generation of photoinduced electrons and holes, which further form radicals whose effects on plastics can be similar to the radicals mentioned above. The goal of this work is to search for new types of photocatalysts for the photocatalytic degradation of microplastics under the influence of visible (solar) radiation. Attention will be focused mainly on metal-free photocatalysts that do not harm the environment and are active under visible radiation.</p>
5	prof. Ing. Kamila Kočí, Ph.D.	Heterojunction photocatalysts for photocatalytic generation of hydrogen	<p>Heterojunction photocatalysts allow to influence the efficiency of the photocatalytic reactions by effective electron-hole pairs separation and permit absorption of incident light to form electron-hole pairs in the solar spectral region. The work will focus on fundamental research on novel heterojunction photocatalysts for photocatalytic hydrogen generation from aqueous solutions of alcohols or other organic compounds. The aim of the work will be a comprehensive analysis of the relationship between the preparation of heterojunction photocatalysts, their physico-chemical properties and photocatalytic activity for hydrogen generation.</p>

6	prof. Ing. Kamila Kočí, Ph.D.	Photocatalytic reactions for environmental protection	<p>Photocatalytic processes are particularly promising for the cleaning of air contaminated by pollutants. By using sunlight they can work even without fossil fuels. One of the key factors influencing the efficiency of photocatalytic reaction is a suitable choice semiconductor photocatalyst that is not only satisfying the energy band gap, but especially desirable position of the valence and conduction bands enabling the successful progress of the process. The main goal of the work is to describe the fundamental facet of the effects on the activity of prepared materials in the photocatalytic reduction of CO₂ and to clarify the relationship between the activity, selectivity and stability of materials and their physico-chemical properties. A trainer's workplace is completely equipped for this job.</p>
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Study program: P0713D070002 - THERMAL ENGINEERING AND FUELS IN INDUSTRY

No.	Supervisor	Title of dissertation thesis	Annotation
1	doc. Ing. Vlastimil Matějka, Ph.D.	The intensification of the separation of the magnetic phases reached on iron presented in slags from steel production	The slags that originate during the steel production processes are reached in iron, which is presented in different phases. Some of these phases have magnetic properties and can be magnetically separated, and the resulting magnetic phase can be used in the process of iron production. The thesis focusses on the search for the optimum process for the isolation of the magnetically active phases from metallurgical slags. The experiments will include the treatment of the slags using selected milling techniques, flotation, and magnetic separation. During the experiments, the magnetic and non-magnetic phases will be achieved, and the emphasis will also be placed on the searching of the application possibilities for both fractions. Obtained samples will be characterised using the methods of chemical and phase analysis, the morphology of the particles will be studied using microscopy techniques.
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	doc. Ing. Marek Velička, Ph.D.	Accumulation of high-potential thermal energy	The topic of the dissertation is focused on the development of materials for high-temperature energy storage systems with high bulk density for the cyclic process of thermal energy accumulation and release. The work will further include modeling verifying the permissible dynamics of the process of charging and discharging thermal energy, the design of geometric shapes of materials and monitoring the influence of boundary conditions on the efficiency of the thermal energy accumulation process.
4	doc. Ing. Hana Ovčáčiková, Ph.D.	Preparation of pigments and glazes from industrial waste	The topic of the dissertation is focused on the characterization of different types of waste across industrial sectors and their potential use as pigment in glazes for ceramic products. The work will include a deeper analysis of potential waste sources, processing and adjustment of pigment granulometry, preparation of a suitable mix of glazes, glazes, determination of colour, determination of basic parameters for pigments and glazes. Design and transfer of material results into practice.
	doc. Ing. Hana Ovčáčiková, Ph.D.	Optimization of 3D printing of ceramic materials	The topic of the dissertation is focused on the use of additive production for the area of silicate materials. The work will primarily deal the optimization of the rheological properties and phase composition of silicate material for 3D printing, adjustment of the composition of the material, granulometric composition and humidity, verification of the effect of special additives and further optimization of the mechanical-physical properties of the material.

			Prerequisites is proposals design of own product, basic orientation in programming and is assumed transferability of results to practice, especially for special products of small series production.
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Study program: P0715D130002 - CHEMICAL METALLURGY

No.	Supervisor	Title of dissertation thesis	Annotation
1	doc. Ing. Kateřina Skotnicová, Ph.D.	Binder systems for diamond grinding tools	<p>The dissertation will focus on the design, preparation and complex characterization of new binder systems based on non-ferrous metals for the diamond grinding tools sintered along the boundaries of diamond grains. Diffusion processes and phase transformations in the systems as Cu-Sn-Ti, Cu-Sn-Co, etc., taking place during the sintering process will be studied in detail. The findings will lead to the development of innovative diamond grinding tools for machining products such as cemented carbides and glass, which will have improved performance, especially lower resistance in machining, improved self-sharpening properties and increased dimensional stability. The structural characteristics, chemical and phase composition of the prepared composite materials will be investigated using scanning electron microscopy, energy-dispersive X-ray spectroscopy, thermal analysis, XRPD, etc.</p>
2	prof. Ing. Jana Dobrovská, CSc.	Study of the kinetics of transformation processes during heating and/or cooling of metallic materials	<p>The kinetics of phase transformations during heating and/or cooling of metals and alloys can significantly influence their microstructure and thus the resulting properties. The dissertation will be focused on the kinetic analysis of selected transformation processes of specified metallic materials based on the non-isothermal and iso-conversional approach. To investigate the phase transformation kinetics experimentally, thermal analysis methods (e.g. Differential scanning calorimetry) will be used to obtain suitable experimental data. These data will subsequently be used in SW Kinetics NEO for modeling the mechanism of transformation kinetics and formal kinetic parameters (activation energy, pre-exponential factor and parameters of the selected model) will be determined. It is assumed that the obtained original results and new findings will expand the field of knowledge in the scientific field of Chemical Metallurgy and related fields.</p>
3	doc. Ing. Vlastimil Matějka, Ph.D.	Study of the nitride phases in steels	<p>The aim of the dissertation is research focused on the determination of nitride phases in steels, modelling of their formation and description of their influence on the properties of selected types of steels. The thermoevolution method will be used to determine nitride phases in selected steels, ThermoCalc and JmatPro software will be used to model the formation, composition and stability of nitride phases. The results obtained by theoretical calculations will be used for the interpretation of the registered thermoevolution curves. The detected presence of given nitride phases will be related to the mechanical properties of the studied steels. The submitted work will be solved in cooperation with Třinecké železářny a.s.</p>

4	Dr. Monika Kinga Michalska	Synthesis and physicochemical characterization of porous carbon composites as electrode material in energy storage application	<p>The main aim of doctoral thesis is to develop the cost-effective methods of preparation of porous activated carbon derived from waste biomass, and its composites with metals or oxides to find an application as electrode materials in batteries and supercapacitors. Green, chemical, and environmentally friendly methods will be implemented as part of this Ph.D. research project. The porous carbon-derived material will be synthesized from biomass waste through thermal carbonization and activation processes using different activating agents. According to physicochemical and electrochemical performances, the impact of pyrolysis temperature will be investigated to determine the proper conditions for the creation of porous carbon material. Afterwards, metals or metal oxides will be used to modify the surface of the carbon-derived materials. The physicochemical techniques, like XRD, Raman, SEM, TEM/HRTEM, BET will support the electrochemical studies. Electrochemical measurements will be performed on the electrode's prepared from these materials to determine the specific discharge capacity, cycleability and high-rate capability.</p>
5	Dr. Monika Kinga Michalska	Synthesis and Characterization of Hierarchical Porous Activated Carbon for Electrochemical Energy Storage	<p>The overall goal of the proposed doctoral thesis is to design cost-effective and scalable methods of synthesizing hierarchical porous activated carbon materials derived from waste biomass for electrochemical energy storage applications. During the realization of the Ph.D. thesis three major objectives will be expected to be accomplished: (1) designing synthesis methods with green chemical and environmentally friendly processes, (2) scaling up of the material synthesis, and (3) their application in solid-state supercapacitors. The hierarchical porous carbon-derived materials will be obtained from biomass waste products purchased from the Silesia-Moravian region via thermal carbonization and activation processes using different activating agents. According to physicochemical and electrochemical properties, the effect of pyrolysis temperature will be investigated to determine the proper conditions for the development of hierarchical porous carbon material. Further, the achieved hierarchical carbon-derived material will be surface modified with metallic nanoparticles. The as-synthesized hierarchical porous activated carbon materials will be studied using several pivotal methodologies, such as X-ray powder diffraction (XRD) combined with Raman spectroscopy, SEM, TEM, HRTEM. In addition, the effect of the electrochemical characteristics will be investigated, and BET measurements will be carried out to control the specific surface area and porosity of the as-synthesized materials. Electrochemical tests will be investigated on the electrodes prepared from hierarchical porous activated carbon materials to ascertain the specific capacitance, energy density, power density, specific discharge capacity, cycleability, and high-rate capability. The device characterization, in the form of solid-state supercapacitors utilizing polymer electrolytes, will be carried out at both the places, Kansas State University and VSB-TUO. The Ph.D. candidate will have an</p>

			international experience to work at both the places as s/he will carried out the proposed thesis research.
6	prof. Ing. Bedřich Smetana, Ph.D.	Synthesis and characterization of new hydrides as effective energy storage materials	The substance of proposed project is a complex experimental and theoretical research in the field of thermodynamical, thermophysical and kinetic behaviour of La-Ni ternary based systems and their quaternar hydrides La-Ni-H. Metallic alloys will be prepared, metallographic, microanalytical and electronmicroscopy analyses (SEM, TEM, EDS, WDS, EBSD) and XRPD/HT-XRPD will be performed. Further key experimental study will be realized using TA methods (TG/DTA, TG/DSC with MS and DILATOMETRY), HP DSC and p-c-T study for hydrogen sorption/desorption study. Experimental part will be supported by theoretical study using ab-initio calculations and Calphad method. The aim of research is obtaining of new knowledge regarding thermodynamical, thermophysical and kinetic behaviour of studied systems, description of relations between studied properties (phase transition temperatures, specific heats, CTE, density,...) and chemical, phase composition and structure in wide temperature region. The research subject is the study of equilibrium phase diagrams and hydrogen sorption/desorption processes.
7	doc. Ing. Vlastimil Matějka, Ph.D.	Synthesis and physicochemical characterization of iron oxides nanocomposites with carbon coatings: Fe _x O _y /C used as electrode materials in batteries and supercapacitors	The main aim of the doctoral thesis is to develop cost-effective methods of preparation of nanocrystalline iron oxides and their nanocomposites with carbon coatings: Fe _x O _y /C of the appropriate structural and electrochemical properties, which find an application as the electrode materials in batteries and supercapacitors. The materials will be synthesized i.e. using modified sol-gel methods, co-precipitation, hydrothermal or combustion methods. Some part of this research work will be focused to create nanocomposites with carbon coatings, i.e. with MWCNT, rGO or g-C ₃ N ₄ . All the synthesized electrode materials will be extensively characterized using several complementary techniques. The crystal structure of the electrode materials will be analyzed by X-ray powder diffraction combined with Raman spectroscopy techniques, the particle size and morphology will be studied by SEM, TEM, HRTEM. Additionally, BET measurements will be used to control the specific surface area and porosity of the synthesized materials. Electrochemical measurements will be performed on the electrode's prepared from the synthesized materials.
8	prof. Ing. Bedřich Smetana, Ph.D.	Study of materials for heat storage and transport technologies	Thesis is focused on the study and development of innovative inorganic materials in solid and liquid phase (liquids and melts) for thermal energy storage, transport and conversion (TES _m - Thermal Energy Storage materials and HTF – Heat Transfer Fluids). Aim of the study is obtaining of modified and new stable progressive materials usable in technological applications (e.g. in the field of CSP - Concentrated Solar Power technologies and in other technological fields) with the potential of more efficient energy storage, transport and conversion. Modification of known and development of new materials with their study will

			be realised for low (below 550 °C) and high (above 550 °C) temperature applications. Experimental study of materials will be realised mainly with use of thermal analysis (TA) and calorimetric methods: DTA, 3D DSC, TG, TG/DTA, TG/DSC a Dilatometry. Theoretical study will be realised also. The subject matter is thermophysical, thermodynamical and kinetic behaviour – properties (behaviour) study of synthesised materials – relation between chemical and phase composition and resulting properties.
9	prof. Ing. Jana Seidlerová, CSc.	Theoretical and experimental study of fine-grained metallurgical wastes recycling	In the context of sustainable development, the use of waste as a secondary raw material is still actual. The amount of collected fine-grain dust increased as a consequence reduction of emission from metallurgical and sinter plants. These dust usually contain more than 20 wt. % of iron and a number of other elements and compounds that can be used in industry. Size of dust particles is the second problem of using material as raw. It is necessary know the method of separation different element and compounds but it is interest study processes how to prepare pellet/briquette and make manipulation with dust easier. Search suitable material for pellet/briquette preparation and study chemical reaction during their processing in metallurgical plants is the topic or dissertation thesis.
10	prof. Ing. Jana Seidlerová, CSc.	Study of organic formation in recycling processes of metallurgical waste	Metallurgical wastes are an important source of iron. However, their recycling is associated with specific problems, including the generation of gaseous pollutants. The work is focused on the study of gaseous pollutants formation depending on the type of both the recycling process and the processed waste under laboratory conditions. Knowledge of the mechanisms and causes of gaseous pollutants formation could contribute to preventing their occurrence.
11	prof. Ing. Bedřich Smetana, Ph.D.	Study and development of materials for heat storage and transport technologies	This thesis is focused on the study and development of innovative materials in solid and liquid phase for thermal energy storage, transport and conversion (TESm - Thermal Energy Storage materials and HTF – Heat Transfer Fluids). Aim of the study is obtaining of modified and new stable progressive materials usable in technological applications (e.g. in the field of CSP - Concentrated Solar Power technologies and in other technological fields) with the potential of more efficient energy storage, transport and conversion. Modification of known and development of new materials with their study will be realised for low (below 550 °C) and high (above 550 °C) temperature applications. Experimental study of materials will be realised mainly with use of thermal analysis (TA) and calorimetric methods: DTA, 3D DSC, TG, TG/DTA, TG/DSC a Dilatometry. Theoretical study will be realised also. The subject matter is thermophysical, thermodynamical and kinetic behaviour – properties (behaviour) study of synthesised materials – relation between chemical and phase composition and resulting properties.

12	prof. Ing. Bedřich Smetana, Ph.D.	Development and study of metal hydrides for chemical energy storage and utilization in the field of hydrogen technologies	<p>The substance of thesis is a complex systematic experimental and theoretical research in the field of thermophysical, thermodynamical and kinetic behaviour of Ca(Co)-Mg-Ni based systems and their hydrides in wide temperature region. Metallographic, microanalytical and electronmicroscopy analyses (SEM, TEM, EDS, WDS, EBSD) will be performed to obtain specified aims. Further key experimental study will be realized using methods of thermal analysis (TG, TG/DTA, TG/DSC with MS, High Pressure DSC and DILATOMETRY). Theoretical study will be performed using thermodynamic modelling by Calphad method. The aim of research is development of new materials for hydrogen storage/release and new knowledge regarding thermophysical, thermodynamical and kinetic behaviour of studied systems, description of relations between studied properties (phase transition temperatures, specific heats, CTE, density,...) and chemical, phase composition and structure in wide temperature region. The research subject is also the study of equilibrium phase diagrams and hydrogen sorption process necessary for utilisation in the field of hydrogen technologies.</p>
13	prof. Ing. Bedřich Smetana, Ph.D.	Study of thermophysical properties of advanced materials based on Fe-C-Mo-Ni-Cr with use of thermal analysis methods	<p>Thesis is focused on experimental and theoretical study of thermophysical behaviour of Advanced alloys by precisely defined conditions. Object of the study are systems in solid and liquid phase (in melt) based on Fe-C-Mo-Ni-Cr, which are important also for technological purpose. Study will be realised mainly with use of thermal analysis methods: DTA, DSC, dilatometry and excelent experimental systems. The relation between chemical composition, phase composition and structural constituents of studied systems and thermophysical properties is one of the work aims. Experimental results will be supported by results obtained with use of thermodynamical SW Thermo-Calc, JMatPro, IDS, possibly with SW Dictra. Creation of own thermophysical and thermodynamical database is assumed. Further aim of the work is the development of methodology of thermophysical properties of materials studied in solid and liquid phase.</p>
14	doc. Mgr. Lucie Bartoňová, Ph.D.	Evaluation of utilization perspectives of industrial wastes	<p>Annually, industrial enterprises produce vast amounts of industrial wastes all over the world. Therefore, further technological utilization of these wastes is a global concern because it not only provides value-added products but also mitigates serious waste disposal problems and, at the same time, facilitates saving natural resources. Industrial wastes exhibit different chemical and physical characteristics depending on their industrial origin and the composition of parent raw materials. For this reason, an optimal utilization approach must be proposed with the view of origin and characteristics of individual waste. To address the aforementioned challenges, the main objective will be to explore the possibilities of utilization of various waste materials and/or their fractions and critical evaluation of corresponding advantages and drawbacks related to their characteristics.</p>

15	prof. Ing. Jana Seidlerová, CSc.	Preparation of slag modification for xenobiotics removal	The topic is focused on preparation and characterization of modified or activated slags that could be used to remove inorganic or organic pollutants. The prepared materials will be tested to use the removal of selected pollutants or groups of pollutants. Modern sophisticated methods of analytical, phase and structural analysis etc. will be used for testing. The determined experimental results will be fitted by suitable physic-chemical models.
16	prof. Ing. Jana Seidlerová, CSc.	Study of organic pollutants formation in recycling processes of metallurgical waste	Metallurgical wastes are an important source of iron. However, their recycling is associated with specific problems, including the generation of gaseous pollutants. The work is focused on the study of gaseous pollutants formation depending on the type of both the recycling process and the processed waste under laboratory conditions. Knowledge of the mechanisms and causes of gaseous pollutants formation could contribute to preventing their occurrence.
17	doc. Ing. Lenka Řeháčková, Ph.D.	Rheological properties of silicate melts and their modeling by artificial neural networks	Adequate slag fluidity is crucial for stable iron production. During this process, crystallization of the slag can occur, accompanied by an increase in its viscosity. The aim of this dissertation is to investigate the influence of the slag composition on the temperature dependence of viscosity. The prepared oxide systems will differ in the content of MgO, B ₂ O ₃ , TiO ₂ , Na ₂ O, CaF ₂ , FeO, and Fe ₂ O ₃ . The measurements will be carried out using an Anton Paar FRS 1600 high-temperature rheometer and will be supplemented by a series of "ex situ" analyses such as electron microscopy and energy-dispersive X-ray microanalysis and X-ray diffraction analysis. The measured temperature dependencies of dynamic viscosity, viscosity and flow curves will be fitted to current models for multicomponent oxide systems, including modeling using artificial neural networks.
18	doc. 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.
19	Dr. Monika Kinga Michalska	Development of high-performance Mg (II) rechargeable batteries for Hybrid Electric Vehicles Applications	The proposal is focused primarily on active electrodes preparation methodologies, structure, and morphology, electrochemical performance of RMBs with and without electrolyte additives to reduce the passivation formation. Detailed structural analyses during cycling will be undertaken using X-Ray Diffraction (XRD), In-situ XRD, scanning electron microscopy and transmission electron microscopy, XPS, Raman, AFM and other related surface studies and secondly is to develop best composite cathodes through 3D electrode architecture for optimum electrochemical performance. DSC measurements will be carried out to clarify the thermal stability and reactivity of the proposed cathodes and anodes in a charged state in the proposed electrolytes.
20	Dr. Monika Kinga Michalska	TMO oxides with activated carbon for energy storage application	The main aim of doctoral thesis is to develop cost-effective methods of preparation of transition metal oxides and their nanocomposites with activated carbon which will find an application as electrode materials in batteries and supercapacitors. During this Ph.D. research project, green chemical and environmentally friendly synthesis methods will be developed. The materials will be synthesized i.e. using modified sol-gel method, co-precipitation, hydrothermal or combustion methods. The particular focus of this study will be to determine the crucial information about the structure, morphology, and electrochemical properties. The effect of the initial heat treatment temperature and atmosphere will also be studied. All the synthesized electrode materials will be extensively characterized using several complementary techniques. The crystal structure of the electrode materials will be analyzed by X-ray powder diffraction (XRD) combined with Raman spectroscopy techniques, the particle size and morphology will be studied by SEM, TEM, HRTEM. Additionally, BET measurements will be done to control the specific surface area and porosity of the as-synthesized materials and the effect of the electrochemical properties will be studied. Electrochemical measurements will be performed on the electrode's prepared from these materials to determine the specific discharge capacity, cycleability and high-rate capability.
21	Dr. Monika Kinga Michalska	Synthesis of porous activated carbon derived from waste biomass as electrode material in energy storage application	The main aim of doctoral thesis is to develop cost-effective methods of preparation of porous activated carbon material derived from waste biomass to find an application as electrode material in batteries and supercapacitors. During this Ph.D. research project, green chemical and environmentally friendly synthesis methods will be developed. The porous carbon-derived material will be synthesized from biomass waste like fruits (i.e., oranges, bananas, apples), vegetables (potatoes, carrots) peels, nuts, and others through i.e., thermal carbonization and activation processes using different activating agents. The effect of

			<p>pyrolysis temperature will be studied to select the best conditions for the formation of porous carbon material according to physicochemical and electrochemical properties. The achieved results will be compared. Later, the achieved carbon-derived material will be surface modified with metals or metal oxides. The as-prepared electrode materials will be characterized using several pivotal techniques, like X-ray powder diffraction (XRD) combined with Raman spectroscopy techniques, the particle size and morphology will be studied by SEM, TEM, HRTEM. Additionally, BET measurements will be done to control the specific surface area and porosity of the as-synthesized materials and the effect of the electrochemical properties will be studied. Electrochemical measurements will be investigated on the electrodes prepared from these materials to determine the specific capacitance, energy density, power density, specific discharge capacity, cycleability, and high-rate capability.</p>
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Study program: P0715D270007 - METALLURGICAL TECHNOLOGY

No.	Supervisor	Title of dissertation thesis	Annotation
1	doc. Ing. Silvie Brožová, Ph.D.	Technological, economic and ecological possibilities of extraction of selected heavy metals from industrial wastes	Metallurgy generates large quantities of metal-bearing waste. Deposition on heaps poses an ecological risk to the environment. The metals contained in the waste represent an economically significant source of secondary raw material. The work will also include the energy benefits of recycling. The aim of the work will be to assess the possibilities of recycling metallurgical waste.
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. Ivo Szurman, Ph.D.	Metallurgical aspects of the preparation of special CCA alloys.	The basis of the dissertation will be the preparation of selected special CCA alloys with the use of vacuum induction melting method. Alloying with a small amount of other elements with the aim of modifying the microstructural characteristics is also assumed. One of the main tasks will be monitoring the metallurgical micropurity of the prepared material. The prepared materials will also be subjected to thermomechanical processing and their microstructural and basic mechanical characteristics will be evaluated using standard methods.
4	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.
5	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.
6	prof. Ing. Radim Kocich, Ph.D.	Design and development of data assembling methodology for rheological law valid for very high strain rates	The aim of these thesis would be in the design and development of methodology leading to achievement of data necessary for chosen mathematical models assembling that describe deformation behavior of chosen materials in broader range of temperatures. For these purposes will be part of work carried out on equipment enabling realization of high speed deformation tests. These aims would be reached also by numerical simulation based on FEM software utilization. Besides, interest will be paid also on the application of newly developed modules aiming to description of phenomenon accompanying these forming processes from view of structure development.
7	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.

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	<p>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.</p>
5	prof. Ing. Daniela Plachá, Ph.D.	Design and synthesis of the single atom with carbon linked covalent organic framework for biomedical application	<p>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.</p>
6	prof. Ing. Kamila Kočí, Ph.D.	CO ₂ transformation to valuable chemicals by photocatalytic processes over highly active materials	<p>The main goal of the work is to describe the fundamental facet of the effects on the activity of prepared materials in the CO₂ transformation and to clarify the relationship between the activity, selectivity and stability of materials and their physico-chemical properties.</p>
7	doc. Dr. Mgr. Kamil Postava	Mueller matrix polarimetry and microscopy of Twisted light	<p>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.</p>

			<p>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 multiphysics) will be used. The modeled structure will be developed by UV laser direct write optical lithography. Methods of Mueller matrix spectroscopy and polarimetric microscopy will be used for optical characterization of the fabricated OEM structures.</p>
8	doc. Dr. Mgr. Kamil Postava	<p>Ultrafast properties of spin lasers with periodic gratings: Novel concepts in data transfer technology</p>	<p>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 optimization 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.</p>
9	doc. Dr. Ing. Michal Lesňák	<p>Application of the SPRi method</p>	<p>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.</p>
10	doc. Dr. Mgr. Kamil Postava	<p>Advanced diffraction optical structures in security holography</p>	<p>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.</p>
11	doc. Dr. Mgr. Kamil Postava	<p>Properties of ultrafast spin-orbit current in magnetic multilayers</p>	<p>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.</p>

12	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.
13	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.
14	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.
15	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.
16	prof. Mark Hermann Rummeli	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, CO ₂ capture and as active electrode material in ion batteries.

17	prof. Mark Hermann Rummeli	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.
18	prof. Mark Hermann Rummeli	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.
19	prof. Mark Hermann Rummeli	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.
20	prof. Mark Hermann Rummeli	Programmed Nanoscale Synthesis of Functional Materials via Electron Beam-Induced Fabrication	<p>This PhD project will delve into the realm of programmed nanoscale synthesis of functional materials, harnessing the power of electron beam-induced fabrication. The research aims to unlock the full potential of electron beams in precisely controlling the creation of advanced materials at the atomic and nanoscale levels. The primary focus will be on developing innovative methodologies, understanding fundamental processes, and exploring diverse applications of these programmable synthesis techniques.</p> <p>Research Objectives:</p> <ol style="list-style-type: none"> 1. Programmable Nanoscale Fabrication: Develop novel strategies and protocols for the precise, controlled synthesis of nanomaterials using electron beam-induced fabrication techniques, such as electron beam lithography (eBL) and electron beam-induced deposition (EBID). 2. In Situ Monitoring and Control: Implement in situ characterization tools within electron microscopes to monitor and control the synthesis process in real-time, enabling adjustments for desired material properties. 3. Materials Diversity: Explore a wide range of materials, including 2D materials, nanoparticles, and nanostructures, with tailored properties for various applications in electronics, photonics, and sensors. 4. Advanced Characterization: Employ high-resolution electron microscopy to characterize

			<p>the synthesized materials at atomic and nanoscale levels, unraveling their structural and compositional details.</p> <p>5. Computational Modeling: Develop computational models to predict and optimize the synthesis of materials, offering insights into the underlying mechanisms and guiding experimental design.</p> <p>6. Applications in Emerging Technologies: Investigate the application of the synthesized nanomaterials in emerging technologies, such as quantum devices, nanoelectronics, and nanophotonics.</p> <p>Expected Outcomes:</p> <ul style="list-style-type: none"> ▪ Pioneering advancements in programmed nanoscale synthesis techniques using electron beams. ▪ A deeper understanding of the in situ control and monitoring of material fabrication processes. ▪ A diverse portfolio of functional nanomaterials with applications in cutting-edge technologies. ▪ High-impact research publications and conference presentations. ▪ Contribution to the development of next-generation electronic and photonic devices. <p>This project offers an exceptional opportunity for a dedicated PhD student to explore the frontier of programmed nanoscale synthesis. It provides the chance to make significant contributions to the field of nanomaterials, fabrication, and their applications in emerging technologies.</p>
21	prof. RNDr. Richard Dvorský, Ph.D.	Preparation of sorption nanostructures with photocatalytic regeneration	<p>Sorbents for water treatment and air cleaning is necessary to replace after saturation and dispose of the exposed material. More economic 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.</p>
22	prof. Ing. Gražyna Simha Martynková, Ph.D.	Membrane composites with nanofibers for the batteries	<p>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</p>

			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.
23	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.
24	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.
25	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.
26	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.

27	Ing. Dominik Legut, Ph.D.	Heat transfer in advanced nuclear fuels	<p>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.</p>
28	Ing. Dominik Legut, Ph.D.	Modelling of THz laser sources	<p>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</p>
29	Ing. Dominik Legut, Ph.D.	Design of novel materials for thermonuclear reactors	<p>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</p>
30	Ing. Dominik Legut, Ph.D.	Multiscale modeling of coupling phenomena in magnetic material	<p>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</p>
31	Ing. Dominik Legut, Ph.D.	Modeling thermodynamic properties of liquid-solid interface	<p>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</p>

			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
32	prof. Ing. Gražyna Simha Martynková, Ph.D.	Application of nanometal particles in conductive polymers for energy applications	<p>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.</p> <p>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.</p>

Study program: P0788D270004 - MATERIAL SCIENCE AND ENGINEERING

No.	Supervisor	Title of dissertation thesis	Annotation
1	doc. Ing. Kateřina Skotnicová, Ph.D.	Structural and mechanical properties of complex concentrated alloys for demanding structural application	The thesis will be focused on the development of precipitation-hardenable complex concentrated alloys (CCAs) based on Co-Cr-Ni-(Al,Ti) and Co-Cr-Fe-Ni-(Al,Ti) with high specific strength for applications in the energy industry, engineering, etc. The kinetics of precipitation of intermetallic particles of type L12 and the effect of high-temperature exposure on the morphology (size, shape and distribution) and volume fraction of precipitates will be studied in detail. Thermodynamic calculations of phase equilibria and phase diagrams using Thermo-Calc will be verified experimentally using DTA, QDS and isothermal annealing. The relationship between the microstructure and mechanical properties of the prepared CCAs will be studied. The deformation behaviour of CCAs during compressive, tensile and creep loading will be studied experimentally.
2	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.
3	prof. Ing. Bohumír Strnadel, DrSc.	The effect of residual stress on fatigue characteristics in structural steels	The study is focused on investigation of fatigue strength of ferritic-pearlitic steels when residual stress acts in microstructure. This effect is investigated in dependence of various parameters in loading such as stress ratio or stress amplitude.
4	doc. Ing. Vlastimil Matějka, Ph.D.	The utilization of the metallurgical slags as the abrasives and fillers in the formulations of friction composites	Slags from the metallurgical industry represent a valuable by-product. Although the effort is to utilise the slags at the highest possible level, some of the slags are still stored in landfills. The implementation of slags as abrasives and fillers in friction composites designed for car brake linings is another way to increase their material utilisation. Within the frame of the Ph.D. thesis, the selected metallurgical slags will be tested as the abrasives and fillers in the formulation of Cu-free friction composites. Several groups of friction mixtures that differ in the type of the slags will be prepared; within these groups, samples with progressively increasing content of the given slag will be prepared as well. Samples in the form of pins will be prepared from the friction mixtures, and their friction-wear performance will be tested using the pin-on-disc tester. The parameters obtained during the testing include friction and wear coefficient; temperature will be related to the character of the friction surface. The

			properties of the primary and secondary contact plateaus will be used to indicate the prevailing character of the friction process, which is the dominant factor affecting the friction-wear performance, as well as the production of wear particles, and is responsible for the comfort properties (noise and vibration) during braking. Selected experiments will be conducted in collaboration with the University of Trento and Lund University.
5	Ing. Martin Négyesi, Ph.D.	Size and shape effects of tested specimens on tensile and fracture properties of structural steels	The knowledge of tensile and fracture properties is necessary for reliable structural integrity assessment. Generally, tensile and fracture properties are measured by standardized tests using standard size specimens. However, a caution needs to be paid when transferring data from laboratory tensile tests to real components with varying sizes and shapes. The so called “size effect” needs to be considered, i.e. tensile and fracture properties are not necessarily independent of the specimen size and shape. Frequently, a lower volume of material is available for testing, so that miniaturized specimens must be manufactured instead of standard size specimens. In such a case, the results of this study may be applied, too. The objective of Ph.D. student will be to examine the influence of specimen size and shape on tensile and fracture test results. Materials under test will be commonly used structural steels. Standardized tensile and fracture testing, light optical microscopy and scanning electron microscopy will be employed in the study. Relationships between microstructural characteristics, such as grain size or precipitates distribution, specimen size and shape and mechanical properties will be searched for. Parameters of micromechanical models, which are based on local approach to fracture, will be found or refined by employing finite element method. All necessary equipment for specimens testing, such as tensile test machine, Charpy impact test machine, light optical and scanning electron microscopes, as well as for specimens manufacturing, such as lathes, CNC milling machine, band saw machines, EDM wire machine, etc. can be found in SIMD (Structural Integrity and Material Design) laboratory.
6	Ing. Martin Négyesi, Ph.D.	The influence of multiple adjoining flaws on structural integrity assessment	The fracture behaviour of structural components caused by single flaw can be well predicted nowadays. However, more adjoining flaws are frequently found in structural components. The adjoining flaws interact together and their resulting effect on the fracture behaviour may become stronger. Estimates of the fracture behaviour caused by adjoining flaws still lack sufficient accuracy. Current criteria are either too conservative or, on the other hand, give non-conservative estimates. The aim of this study is to shed more light on the issue of adjoining flaws and contribute to the refinement of the current criteria. Effects of the distribution and sizes of the adjoining flaws on the fracture toughness will be investigated. New fracture criteria will be proposed and parameters with major role on the flaw growth will be identified based on the results of this study. The study will also deal with specimen

			<p>manufacturing which is challenging and needs a special technique to be employed. Steel plate specimens with surface or through-thickness flaws will be preferentially tested. Specimens will be introduced into tensile and bend testing with monotonic loading. The effect of microstructure on the growth of adjoining flaws will be also treated by employing the fractographic analysis. FEM analyses will be used in order to reduce the number of experiments. All necessary equipment for specimens testing, such as tensile test machine, light optical and scanning electron microscopes, as well as for specimens manufacturing, such as lathes, CNC milling machine, band saw machines, EDM wire machine, etc. can be found in SIMD (Structural Integrity and Material Design) laboratory.</p>
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