PROJECTS OF THE INSTITUTE OF MATERIALS SCIENCE

Project Title	**Design and preparation of high-temperature superconducting tapes joints using lead-free solders and characterization of their properties**
Coordinator	Dr. Ing. Marcela Pekarčíková
Start Date	01/01/2017
End Date	31/12/2020
Program	VEGA
Annotation	This project of fundamental research is aimed to design and preparation of functional joints made of high-temperature superconducting tapes using lead-free solders based on tin or other low-melting elements. A conventional and induction soldering will be used for preparation of the joints and suitable parameters of joining process should be found by optimization methods. Development of microstructure, electrical and mechanical properties will be studied in prepared joints. Achieved results will be published in CC journals and presented on world-level scientific conferences.

Project Title	**The effect of microstructure and phase composition on corrosion resistance of hot dip alloys**
Coordinator	doc. Ing. Martin Kusý, PhD.
Start Date	01/01/2018
End Date	31/12/2021
Program	VEGA
Annotation	The submitted project focuses on the detailed study of microstructure and phase composition of Zn and Al alloy for hot dip coatings. Microstructural characteristics, changes in phase composition, solid solution supersaturation and texture will be analyzed in relation to the resistance of the analyzed corrosion resistant alloys. The alloys will be prepared by rapid solidification processes in bulk, suitable for more complex microstructural analyzes, but also in the form of thin coatings made by dipping in molten alloys. The rapid solidification as an alloy preparation process was chosen because of the similarity with the hot-dipping processes on the continuous production lines. We study in detail the simple system based on the reactive diffusion couple Fe-Zn, which we describe in after equilibrium and non-equilibrium solidification via suitable thermodynamic models using the Calphad method. These will then be used to model the microstructure by the Phase Field method implemented in the Micress program.

Project Title	**Materials design of high-entropy alloys and their characterization**
Coordinator	RNDr. Pavol Priputen, PhD.
Start Date	01/01/2018
End Date	31/12/2021
Program	VEGA
Annotation	The goal of the work is to design and prepare series of high-entropy alloys in the form of bulk alloys, as well as thin films and to do basic characterization of their structure, phase constitution and properties. The bulk alloys will be prepared by arc and/or induction melting, while the thin films will be prepared

by magnetron sputtering and ion implantation. For structure and phase constitution analysis, electron microscopy, x-ray diffraction, electron diffraction, and energy dispersive x-ray spectroscopy techniques will be used. Among the properties studied, the attention will be focused particularly on mechanical properties (hardness, toughness and strength), chemical properties (corrosion resistance), and physical properties (thermodynamic stability). The project is oriented on fundamental research with regard to practical applicability of the results achieved. Obtained findings will be published in in peer-reviewed journals from CC database and presented at international scientific conferences.

Project Title	**The physical properties of disordered structures influenced by accelerated ions**
Coordinator	prof. Ing. Marian Kubliha, PhD.
Start Date	01/01/2018
End Date	31/12/2020
Program	VEGA
Annotation	The project is aimed at the studying the influence of structure and physical properties of special glasses and rubber compounds on accelerated ions. In the area of glasses based on chalkogenides and heavy metal oxides,the aim is to prepare materials with a locally enhanced dopant which is difficult to achieve by preparing using melt cooling method. From a technical point of view, there is mainly characterization of application interesting optical,luminescent and electrical properties. In the field of rubber compositions, objective is to characterize the irreversible changes of the structure (crosslinking, degradation) induced by accelerated ions. In terms of expertise, this is in particular a qualitative and quantitative characterization of changes in the structure and properties of irreversible chemical reactions.

Project Title	**Research of possibilities of Al-Ti-N based hard coatings thermal oxidation stability enhancement**
Coordinator	prof. Ing. Ľubomír Čaplovič, PhD.
Start Date	01/01/2019
End Date	31/12/2021
Program	VEGA
Annotation	The project is focused on a development and characterization of hard coatings produced for tool materials and characterized with enhanced thermal and oxidation resistance. It is based on the current knowledge in the field of influence of alloying elements such as B, La, V, Ta and W on increasing of Ti-Al-N coatings oxidation resistance. Two technological processes (cathodic arc vacuum and magnetron sputtering) will be involved for depositions of functional coatings and evaluation of alloying elements effect on increasing of thermal resistance and nanostructured morphology of such fabricated coatings. The most advanced analytical techniques, such as HRSEM, HRTEM, EBSD, XRD, PIXE, RBS and tribological tests will be used for coatings characterization. The aim of the project is a development of new advanced

coatings designated for tool materials and characterized with excellent tribological and thermal properties

Project title: **Determination of optimal cryogenic treatment regime for tool steels**
Coordinator: prof. Ing. Peter Jurči, PhD.
Start date: 01/01/2020
End date: 31/12/2023
Programme: VEGA
Annotation: The projekt is focused to in-depth investigation of phenomena that occur in selected chromium-vanadium ledeburitic tool steel as a result of different regimes of cryogenic treatmnent. Effects of important processing variables like the austenitizing temperature, temperature and duration of sub-zero treatment, and tempering regimes on the microstructure, hardness, flexural strength, fracture toughness, wear performance and corrosion resistance of examined steel will be determined within the project. This woiuld lead to better exploitation of the potential of cryogenic treatment for tool steels. A great number of experimental techniques will be used in the project, which enables to achieve the main scientific goal – to confirm the scientific hypothesis on possible simultaneous enhancement of normally conflicting properties like hardness and wear resistance on the one side, and the toughness on the other side, for selected Cr-V ledeburitic steel by using the cryogenic treatment.

Project title: **Physical properties of heavy metal oxide glasses**
Coordinator: Mgr. Ondrej Bošák, PhD.
Start date: 01/01/2020
End date: 31/12/2022
Programme: VEGA
Annotation: The project is focused on the study of special glasses designed for applications in photonics and optoelectronics including the central area of the infrared area of the spectrum. New ternary glasses based on TeO2 and Sb2O3 will be prepared on the basis of international cooperation. In the first part, selected physical properties of glasses will be characterized. In the framework of the project solution, effects of changes in the glass composition, observable changes in structure, and the possibilities of rare earth elements doping will be investigated by using electrical and dielectric methods. The next part will examine the influence of technological parameters of glass preparation, possibilities of diagnostics and prediction of achieved quality by monitoring of selected electrical parameters.

Project title: **E-learning and implementation of information technologies in teaching of materials-technology courses**
Coordinator: doc. Ing. Roman Moravčík, PhD.
Start date: 01/01/2020
End date: 31/12/2022
Programme: KEGA
Annotation: The project is focused on the implementation of e-learning in the teaching and examination process in materials-oriented courses such as Materials Science I,

Mechanical Testing and Defectoscopy of Materials, Heat Treatment and Surface Treatment of Materials and Thermodynamics and Kinetics, taught at the Faculty of Materials Science and Technology in Trnava, Slovak University of Technology in Bratislava (MTF STU).

Project title: **Development of the Fe based PM components with increased fatigue strength.**

Coordinator: doc. Ing. Martin Kusý, PhD.
Start date: 01/07/2019
End date: 30/06/2022
Programme: APVV
Annotation: The problem of the current serial production of PM-based Fe parts in the case of uniaxial single compression in combination with sintering, calibration and heat treatment for commercially used powder mixtures (in particular FeCu1.8C0.7 and FeMo0.5Ni0.5C0.6) is its density in range 6.9 -7.1 g.cm-3. In the case of the use of such components for the "high-performance" applications in engines and transmissions where resistance to dynamic load, high strength or fatigue properties is required, residual porosity is a limiting factor. The aim of the present project is therefore to develop PM-based Fe parts with a higher density > 7.4 g.cm-3 in series production to reduce porosity (mainly open and bonded pores) and its potential use in "high-performance" applications. With regard to the manufacturing infrastructure of Miba Sinter Slovakia Ltd. (subcontractor of the project), it is necessary to examine in detail the impact of the modification of the powder mixture (with respect to the amount of lubricant) and compression parameters (pressure and velocity) on residual porosity and fatigue strength. However, production technology must be designed with respect to the quality of the die, which is currently designed to working pressure up to 600 MPa.

Project title: **Study of non-conventional glasses modified by ion exchange or ion implantation**

Coordinator: Mgr. Ondrej Bošák, PhD.
Start date: 01/02/2020
End date: 31/12/2022
Programme: APVV
Annotation: The proposed project deals with the modification of surface of chalcogenide glasses by Na and K cations doping in order to modify their refractive index and/or their electrical conductivity. Glass samples will be prepared, modified by ion exchange or ion implantation and next they will be tested for their optimal functionality. Electrical and dielectrical properties will be used for characterization of ion content and transport in the investigated glasses. Analyses will be focused on the so-called phenomenon mixed-alkali effect. Surface of glasses prepared by ion implantation will be analyzed by RBS/ERDA and PIXE spectroscopy.

Project title: **Preparation and chracterisation of disordered materials for aplication in infrared spectra**

Coordinator: doc. RNDr. Vladimír Labaš, PhD.
Start date: 01/03/2020
End date: 31/12/2022
Programme: APVV
Annotation: Project is oriented on support of scientific cooperation of institutes from four contries and education of Ph.D. students in the field of special glasses. By using international cooperation, new glass systems based on chalcogenides and heavy metal oxides will be prepared. The thermal, optical, structural and electrical properties of prepared glass systems will be analysed using instrumentation of all partners. The influence of technological parameters on the chalcogenide glasses with gradient chemical composition influenced by gamma radiation as well as on selected glasses based on heavy metal oxides, will be studied. The possibilities of diagnostics of investigated glasses will be verified by monitoring of selected electrical parameters.

Project title: Cost effective FCL using advanced superconducting tapes for future HVDC grids
Coordinator: Ing. Dr. Marcela Pekarčíková
Start date: 01/01/2017
End date: 30/06/2020
Programme: H2020
Annotation: Sustainability of energy systems goes through high penetration of renewable energy with huge volumes of electricity to transmit over long distances. The most advanced solution is the HVDC Supergrid. But fault currents remain an issue even if DC circuit breakers have emerged. These are not satisfying, whereas Superconducting Fault Current Limiters (SCFCLs) using REBCO tapes bring an attractive solution. SCFCLs have already proved their outstanding performances in MVAC systems, with a few commercial devices in service. However,present REBCO conductors cannot be readily used at very high voltages: the electrical field under current limitation is too low and leads to too long tapes and high cost. FASTGRID aims to improve and modify the REBCO conductor, in particular its shunt, in order to significantly enhance (2 to 3 times) the electric field and so the economical SCFCL attractiveness. A commercial tape will be upgraded to reach a higher critical current and enhanced homogeneity as compared to today's standards. For safer and better operation, the tape's normal zone propagation velocity will be increased by at least a factor of 10 using the patented current flow diverter concept. The shunt surface will also be functionalized to boost the thermal exchanges with coolant. This advanced conductor will be used in a smart DC SCFCL module (1 kA - 50 kV). This one will include new functionalities and will be designed as sub-element of a real HVDC device. In parallel to this main line of work, developments will be carried out on a promising breakthrough path: ultra high electric field tapes based on sapphire substances. FASTGRID will bring this to the next levels of technology readiness.

PROJECTS OF THE INSTITUTE OF PRODUCTION TECHNOLOGIES

Project Title	**The research of light alloys joining by progressive methods take into consideration of environmental suitability and quality tested by modern NDT methods**
Coordinator	doc. Ing. Erika Hodúlová, PhD.
Start Date	01/01/2017
End Date 3	31/12/2020
Program	VEGA
Annotation	The literature research based on the current state of the light alloys application, especially in biomedicine,aerospace and automotive industries are the project aims the basic research of oints creation from the light alloys by the advanced joining techniques in assurance of quality and environmental suitability. The research will focus on the joining of pure materials (Ti, Mg, Ni and Al), its alloy and its combination. The joints will be created by the beam technologies (laser and electron beam), diffusion bonding by using the reactive interlayers and the combination of environmentally friendly solders and reaction layers materials using for joining. The quality of the joints will be tested using the sophisticated destructive and non-destructive methods. Research will be focused on the control of technological parameters affecting the joining process stability and repeatability at the using of high speed joining velocity of joints free of defects.

Project Title	**The research of novel method for cutting edge preparation to increase the tool performance in machining of difficult-to-machine materials**
Coordinator	Ing. Tomáš Vopát, PhD.
Start Date	01/01/2017
End Date 3	31/12/2020
Program	VEGA
Annotation	Cutting edge preparation is that the appropriate micro-geometry of the cutting edge is essential for achieving high productivity of the particular difficult-to - machine and tough materials such as austenitic stainless steels and superalloys. It also suggests a larger deployment of superalloys in the coming years. The proposed project is focused on research into new methods for edge preparation and cutting edge: plasma polishing in an electrolyte (PPE). Comparing the tool life of cutting tools preparared by the same method with different radii of curvature of the cutting edge of the tool will be found suitable size to machining tough materials and dificult-to-machine. By applying these results in the production of instruments to extend their life, saving the cost of the tool during operation. Comparing the durability of cutting tools prepared by new method PPE with selected industrial methods with the same radius of curvature of the cutting edge will be found applicability of test methods PPE.

Project Title	**Optimization of geometry of cutting tools produced by foundry technology and powder metallurgy to increase durability**
Coordinator	prof. Ing. Alexander Čaus, DrSc.
Start Date	01/01/2019
End Date	31/12/2022

Program VEGA

Annotation Geometry of cutting edge has significant effect on wear resistance as well on durability of cutting tools. It is possible to produce near-net-shape cutting tools by both the foundry technology and the powder metallurgy and in the case of high speed steel (HSS) with significantly higher wear resistance compared to similar tools produced by conventional metallurgy using machining of wrought profiles. Optimization of cutting tool geometry will be carried out by numerical simulation of machining conditions and load for the tool in cutting process. Application of additive technologies, namely 3D printing of casting patterns from castable resin for investment casting into ceramic shell moulds, and cemented carbides (CC) from metal powder, provides flexible production of cutting tools with optimal shape without using very expensive and shape-complicated injection moulds for production of castable/burnout casting patterns as well as for forming dies for powder material compaction.

Project title: Coating of powder metallurgical Titanium using electromagnetic radiation under working atmosphere, study of microstructure and coatings properties

Coordinator: prof. Ing. Peter Šugár, CSc.

Start date: 01/01/2020

End date: 31/12/2022

Programme: VEGA

Annotation: The project deals with the possibility of surface treatment of titanium, which was prepared from titanium powder by low temperature methods of powder metallurgy. It is envisaged to use an energy beam of electromagnetic radiation incident on the surface of the PM titanium either in the form of laser beam or in the form of focused solar radiation. When heated under the working atmosphere, the reaction of titanium with oxygen or nitrogen molecules is assumed and coatings based on oxides, nitrides or their mixtures are expected to be formed. Subsequently,the microstructure and selected properties of the prepared coatings will be studied. The aim is to explore the possibilities of surface treatment of PM titanium, depending on future applications, to prevent surface damage during friction, to improve the surface for biocompatibility and to increase corrosion resistance of PM Ti, which are the most important reasons for surface treatment of usual titanium components.

Project title: Accurate calculations, modeling and simulation of new surfaces based on physical causes of machined surfaces and additive technology surfaces in machinery and robotical machining conditions

Coordinator: Dr.h.c. prof. Ing. Pavol Božek, PhD.

Start date: 01/01/2020

End date: 31/12/2022

Programme: VEGA

Annotation: The central idea of the project is to use accurate calculations based on analytical equations as a basis for predicting roughness characteristics of machined surfaces. At the center of interest are the physical causes of machined surfaces studied at the level of geometrical-kinematic, mechanical-physical and technological properties of members of the machining system. Our intention is

to create mathematical models and simulation algorithms for individual physical causes of the machined surface. As study prototypes, we will consider type-defined and undefined cutting edge technologies and exception-additive technology. Another target group of research is the inclusion of significant dynamic and stiffness characteristics. machines and machining robots. It is in robots that more time and emphasis will be placed on studying the effects of motion, kinematic bonds and trajectories. The inclusion of a robot technology and additive technology system is an important element of our research as a central project note.

Project title: **Research of joining the metallic and ceramic materials in production of power semiconductor**

Coordinator: prof. Ing. Roman Koleňák, PhD.
Start date: 01/01/2020
End date: 31/12/2023
Programme: VEGA
Annotation: The project is aimed to fundamental research of solderability of metallic, composite, non-metallic and ceramic materials applied in packaging of power semiconductor parts (chips, transistors, diodes etc.). The solution will be oriented to direct joining without application of coating for wettability assurance. Joining of semiconductor materials as Si, SiC and GaN is considered. Furthermore Al2O3, Si3N4, AlN and Cu/SiC composite material, which is applied mainly for the cooling of chips are also taken into account. Cu will be applied as an etalon material. New solder alloys alloyed with a small amount of active elements (Ti, La etc.) will be manufactured and also the solder alloys containing Bi and Zn, applicable for higher service temperatures. The solders will be designed with the aim to be suitable for direct soldering with application of power ultrasound. These new solders will be then tested for technological solderability. The interactions of solder alloys with the surface of substrates will be studied.

Project Title **Specialised laboratory supported by multimedia textbook for subject "Production systems design and operation" for STU Bratislava**

Coordinator Dr. h. c. prof. Ing. Pavol Božek, CSc.
Start Date 01/01/2018
End Date 31/12/2020
Program KEGA
Annotation The project proposal submitted is oriented on creating a new laboratory supported by the multimedia university textbook for teaching a new subject "Production systems design and operation" in both written and interactive formats due to possible continuous complementation/ upgrade and improvement of specialised knowledge related to production systems as well as to their control systems at higher education. The support of improved, more intensive and efficient perception of information from the printed textbook for the subject of „Production systems design and operation" (i.e. texts, figures, graphs, talk, animations, videos) is provided via multimedia allowing thus their showing in more versions. Videos supporting the written information will

complement individual chapters and parts of the aforementioned higher education textbook. Multimedia possibilities as well as hypertext are the right tool for supporting specialised study information providing easy browsing in the book and user-friendly orientation within. The basic principles of selected process technology systems will be executed also via a specialised laboratory for the subject in question. The introduction to each chapter of this multimedia textbook will be complemented by key words both in Slovak and English languages. The conclusion of each chapter will be complemented by an interactive test.

Project Title	**Development of a laboratory for the design and maintenance of production systems supported by the use of Virtual Reality**
Coordinator	doc. Ing. Peter Košťál, PhD.
Start Date	01/01/2018
End Date	31/12/2020
Program	KEGA
Annotation	The presented project focuses on the topic "New Technologies, Methods and Forms in Teaching" with a special focus on new methods and forms of education at universities and on the development of key cognitive operations, e.g.: knowledge, capacity, skills and habits to just cite a few. All this in the frame of the preparation of new educational programs in specialized laboratories. The main objective of the project is to introduce an innovative way of educating and preparing students and with this contribute to the formation of high-quality professionals who are competitive on the European labor market and Slovakia itself.

Project Title	**Multimedia tools for teaching foundry technology and its content optimization in the countries of the Visegrad group**
Coordinator	doc. Ing. Štefan Podhorský, CSc.
Start Date	01/01/2018
End Date	31/12/2020
Program	KEGA
Annotation	Enable to optimize the content of subjects of foundry technology on the basis of experiences acquired from teachers of the Visegrad group countries. The teaching tools will be proposed and created for more attractive learning and easier exchange trips of students between universities of Visegrad group countries. It will also prepare graduates of universities for job market in these countries. The optimized content of learning will enable students to acquire similar knowledge from area of foundry as graduates form any other countries of the Visegrad group.

Project title	**Modern educational tools and methods for forming creativity and increasing practical skills and habits for graduates of technical university study programmes**
Coordinator	Dr. h. c. prof. Ing. Pavol Božek, CSc.
Start date	01/01/2019
End date	31/12/2021

Programme: KEGA

Annotation: 4th Industrial Revolution (Industry 4.0) covers a wide range of large-scale and mass production in Slovakia. At present, the automotive industry is the dominant industry in Slovakia. So far, we have just been a "workshop", with no added value. Unfortunately, technical programme graduates at universities have neither the qualitatively nor quantitatively the required creativity and practical skills and habits to be applied in the companies involved. For manufacturing companies, however, it is necessary to educate a new generation of educators and students who will understand these technologies and know how to use them. This project offers the methodology and tools that are absolutely necessary to be implemented in the educational process in the technical study programmes at Slovak universities. This is mainly about a transfer of newly acquired knowledge from current research and views at contemporary manufacturing businesses in line with industry 4.0 requirements. In this context, it will be very important to include practical lessons in educational process with clearly defined conditions and a defined evaluation methodology. The project considers the use of knowledge based on the literary resources analysis from the creativity forming area of students of technical study programmes using modern educational tools and technologies. At the same time, the approach will be used, followed by synthesis in the formation of creativity and the enhancement of practical skills and abilities of technical study programmes graduates. The practical verification of the selected methods will be realized by applying modern educational tools with a connection to the real requirements of the production practice.

Project title **Modernisation of education in the area of joining of engineering materials**

Coordinator prof. Ing. Milan Marônek, CSc.

Start date 01/07/2019

End date 31/12/2021

Programme: KEGA

Annotation: The project focuses on the design and implementation of a new concept of study literature creation with regard to the demands and expectations of the current young generation (Generation Z). The proposed concept will support the implementation of multimedia content that greatly helps to facilitate understanding of the issue and reflects the behavioural characteristics of the young generation that is essentially linked to Internet content and social networks. The concept is based on the creation of information database on the progressive joining of materials available online in one place. In each theme, there will be a technology principle, equipment description, explanation of the technological parameters, practical applications of technology and visual demonstrations in the form of animations, videos and pictures.

Project title **Improving profesional competences of the university graduates of the branch Manufacturing Technology by applying dual education principles**

Coordinator prof. Ing. Peter Šugár, CSc.

Start date 01/07/2019

End date 31/12/2021

Programme: KEGA

Annotation: The projects solves the conceptual, methodological and content issues of the second grade university education in the Production Technologies study programme with the aim of more intensive developing of the graduates professional competences and their ability to fulfill the requirements of modern manufacturing practice. The expected output of this project is to upgrade the existing model of the student education in the Machining and Forming study programme by implementing the elements of dual and online asynchronous e-learning system. The definition and the verification of the practical training methodology and the content will be implemented in terms of the industrial partners. At the same time, the project output also will be the development of an integrated e-system for an education and the management of praxis-orientated educational activities together with the establishment of the conditions for the face-to-face laboratory trainings focusing on the development of the creative solution for the actual and verifiable-by-praxis tasks. The tasks will be solved in the field of production technologies and the company process management, taking into account the need to quickly adapt the graduate to the bilingual business environment.

Project Title **Creation of new study materials including multimedia textbook in field of technical preparation of production in welding and joining**

Coordinator prof. Ing. Roman Koleňák, PhD.

Start Date 01/01/2020

End Date 31/12/2022

Program KEGA

Annotation The project is focused on the design and creation of a new modern university textbook and didactic tools for teaching the subject: "Technical preparation of production in welding and joining materials". The subject is part of a new study program at the MTF STU entitled "Welding and Joining Materials", to which there are no suitable teaching texts or other didactic tools in historical context. The proposed concept is aimed to creating a textbook and an electronic version of a textbook with multimedia content. The creation of new study materials will directly influence the understanding of the issue under consideration in order to prepare graduates for the profession of welding technician as well as technician in engineering. The textbook will contain the materials needed to understand the technical documentation of welding and bonding. Understanding the preparation and implementation of the documents needed before, during and after the release of the engineering product to production is very important in terms of time and quality. The accompanying product is the creation of multimedia content, which will include a chronological approach to creating technical and welding documentation with explanations of operations using graphical representations and practical examples. The aim of the course is to prepare a student who is able to prepare materials for the construction of connected structures from the breakdown of materials through their security, storage, labeling, distribution to individual workplaces for preparatory operations and their progress to the final workplace for joining parts to individual nodes and units.

Project title	**Research of technological process of forming at production of tubes with contoured internal surface**
Coordinator	prof. Ing. Maroš Martinkovič, PhD.
Start date	01/07/2016
End date	30/06/2020
Programme	APVV
Annotation	It is necessary to pay close attention to the research of deformation processes regarding the production of seamless cold drawn tubes, whether precision tubes or tubes with contoured internal surface for industrial purposes. Rationalization of production requires to analyze state of stress and deformation at different methods of tube drawing (drawing on a cylindrical plug, drawing on a floating plug, drawing on a rod, drawing by die move - without plug), with special attention to the question of possible development of finished products (precision tubes) by increasing the intensity of industrial moves (maximum reduction) as well as the feasibility of multistage drawing (i.e. incremental forming) without inter-annealing. Microstructural analysis will be used for plastic deformation of individual moves in the tube volume, the analysis of limit plasticity state, when drawing of tubes tends to increase the dislocation density up to its critical level, which represents immobility of dislocation, i.e. termination of the material deformability with subsequent damage (rupture) of material. Experimental processes will be numerically simulated in a virtual environment of DEFORM 3D program, numerical models will be verified by comparison with experimental results of microstructural analysis and dimensional analysis using computer tomography, Consequently the research results will be verified in practice.

Project Title	**Research into the Unique Method for Treatment of Cutting Edge Microgeometry by Plasma Discharges in Electrolyte to Increase the Tool Life of Cutting Tools in Machining of Difficult-to-Machine Materials**
Coordinator	prof. Ing. Alexander Čaus, DrSc.
Start date	01/07/2017
End Date	30/06/2021
Program	APVV
Annotation	The cutting edge preparation (CE) is currently the most advanced method of increasing tool life. Cutting edge preparation in the production of cutting tools means treatment of microgeometry of cutting edge (cutting edges) of newly sharpened cutting tools. Suitable microgeometry of the cutting edge (fillet, chamfer) is essential for achieving high productivity machining mainly difficult-to-machine materials (DTM) such as austenitic stainless steels and superalloys. Therefore, the research deals with the machining of X6CrNiTi18-10 stainless steel and NiCr19FeNbMo superalloy. Machining superalloys disseminate knowledge in the energy and aerospace industries since it requires a greater commitment superalloys in future years. Our proposed project is focused on research into a completely new and own unique method of preparation of CE microgeometry of cutting tools by plasma discharge in an electrolyte (PVE). This

method is developed originally at Faculty of Materials Science and Technology in Trnava, Slovak University of Technology in Bratislava (STU MTF).

Project Title	**Research of direct bonding of the ceramic and metallic materials by use of active soldering alloys**
Coordinator	prof. Ing. Roman Koleňák, PhD.
Start date	01/07/2018
End Date	30/06/2022
Program	APVV
Annotation	The project deals with the study of direct bonding of ceramic and metallic materials by application of active soldering alloys. The active alloys will be based on tin or indium and alloyed with active metal, as for example Ti, La, Zr, Y etc. It is supposed that the active element will react with the substrate surface during soldering process and will thus assure the wetting of solder on a ceramic or other hard-to-solder material. The project is based on idea of direct fluxless bonding. Heating will be provided by the high-concentrated heat sources as the laser and electron beam. Power ultrasound will be employed for activation of the new soldering alloys. Material solderability of the new developed solders will be studied. The following solderability criteria will be determined: wettability, spreadability, diffusion etc. Also interactions on the substrate/solder interface will be studied. Individual mechanisms of bond formation from the viewpoint of joint strength, speed of bond formation, life etc. will be compared.

Project Title	**Research of progressive methods of welding and soldering of corrosion-resistant steels and copper**
Coordinator	doc. Ing. Erika Hodúlová, PhD.
Start Date	01/07/2019
End Date	30/06/2023
Program	APVV
Annotation	The proposed project will be solved as a scientific research project focused on basic research in the field of welding and brazing/soldering of stainless steel with copper alloy by technologies utilizing progressive joining methods of materials. Several modern scientific methods will be used within the project in order to fill up the objectives set in particular stages of the project. In the early stages of the project, method of scientific analysis and planning of the experiments using Design Expert software package will be used to determine the optimal parameters of high-productive joining methods (laser beam, electron beam, CMT, brazing/soldering) of the two types of joints (butt joint and lap joint). To achieve the stated objectives working procedures will be developed based on the knowledge and gathered information. Macrostructural and microstructural analysis of the joints will be used as experimental methods to evaluate the structural integrity of welded and brazed joints. EDX analysis and extended to high-resolution transmission electron microscopy will be used to determine creation of different phases and change in chemical composition as well as the dentification of excluded phases in joints. For the determination of internal defects of welded joints the computer tomography will be involved.

The mechanical properties of the joints will be evaluated by tensile strength test in case of butt welds, by shear strength in case of lap joints, micro-hardness and bend test.

Project Title	**Research of progressive methods of welding and soldering of corrosion-resistant steels and copper**
Coordinator	doc. Ing. Ladislav Morovič, PhD.
Start Date	01/07/2019
End Date	30/06/2023
Program	APVV
Annotation	The shape stability of the steel tubes has a major influence on the further technological process of the tube processing, i. e. on secondary production. It is a very important parameter in terms of functionality, for example, active and passive parts of a car, where the dimensional tolerance fields are one of the toughest in terms of prodution itself. It is important to pay attention to the research of the shape stability of the tubes by means of contact metrology systems (coordinate measuring machine with touch probe) and non-contact measuring systems (optical 3D scanner using active triangulation (structured light)). The resulting properties of the tubes depends on a number of factors, e.g. from the shape instability in the individual phases of the production process in the process of production of tubes in Železiarne Podbrezová. The shape stability and the occurrence of geometric deviations are affected by the eccentricity that occurs primarily in the perforation process due to the off-centered punch, where there is uneven distortion due to the change in the original cross-sectional area of the blank on the radial removing of the material. In the process of producing tubes at the tensile reduction, a polygon is formed which results in uneven deformation caused by the stands in which the rolls are placed. Uneven distortion affects the internal structure of the material and hence the shape stability in the subsequent operation due to the anisotropy of properties. Experimental processes will be numerically simulated in the software DEFORM 3D. The aim is to identify, quantify and subsequently determine the effect of geometrical deviations on the instability of the tube dimensions and their technological inheritance, which is supposed to meet the most stringent technical and supplier conditions for the industry.

Project Title	**Prototype development of an industrial device for electrolytic-plasma polishing of parts of lung ventilators and other medical devices**
Coordinator	doc. Ing. Štefan Podhorský, CSc.
Start Date	16/09/2020
End Date	31/12/2021
Program	APVV
Annotation	The surface of products intended for biologically active environments must meet significant quality requirements. This also applies to parts of the lung ventilators. Low surface roughness is required because the ability of microorganisms to be trapped on a smooth surface is significantly worse than on a rough surface. Microscopic defects of the surface layer of the material have a significant negative effect, as well, which represent a significant risk

factor not only in terms of possible biological contamination of the surface, but also in terms of microbiological corrosion. Although mechanical polishing methods reduce the surface roughness, they effect on the surface by force and heat, creating a number of microscopic defects that are usually furthermore contaminated with impurities during polishing. Therefore, it is common practice to polish the surface of such products electrochemically, but this necessitates the use of aggressive substances, usually a mixture of concentrated corrosives. Disposal of used solutions, containing a lot of dissolved metals, means a significant environmental and financial burden. An ecologically and technologically advantageous alternative to electrochemical polishing is a unique technology of plasma polishing in electrolyte, which is still relatively unknown worldwide. The team of the research laboratory has been devoting a long time to the development of this progressive technology, but the most significant obstacle to its introduction into industrial practice is the non-existence of equipment that would be directly usable in the production process. The goal of the presented project is to solve this problem. The aim of the project is the development of technological equipment for plasma polishing in electrolyte and the realization of a prototype.

PROJECTS OF THE INSTITUTE OF INDUSTRIAL ENGINEERING AND MANAGEMENT

Project Title	**Proposal of the combination and recombination methodology for the work comfort index in mechanical engineering industrial plants**
Coordinator	doc. Ing. Alena Paulíková, PhD.
Start Date	01/01/2018
End Date	31/12/2020
Program	VEGA
Annotation	In engineering operations, the assessment of workload in most cases is still discretionary. Assessment usually takes place without determining the interdependence of the effects of individual factors on the body of the exposed worker during his / her work. The presented project is aimed at designing a procedure for expressing the synergic effect of occupational comfort factors, which would allow their mutual combination and recombination by type of operation and age category. The aim of the project is to define the "work comfort index" as a comprehensive indicator of the effects of monitored and measured factors of the working environment in engineering operations. The Work Comfort Index allows individual workload adjustment and work environment for employees in engineering operations to ensure their stable performance with the highest possible safety and health protection.

Project Title	**Big data analytics as a tool for increasing the competitiveness of enterprises and supporting informed decisions.**
Coordinator	doc. Ing. Helena Makyšová, PhD.
Start Date	01/01/2018

End Date 31/12/2020
Program VEGA
Annotation The key to the effective use of information is the design of a suitable model of their exploitation defining all activities, also covering the creation of predictive models as a source of informed decisions at the management or process level. Choosing the right data mining method is currently a problem because there is not a comprehensive concept describing the causal relationship (if any) between the problem structure and the properties of the method. Up to now, the cases outlined in the literature are so- called Ad-hoc solutions. Therefore, the presented research project would like to examine the existence of causality between the characteristics of the data sets and the usability of the available methods, to formalize the acquired knowledge and thus to create the preconditions for their digitization. The proposed solution will be experimentally verified in the field of logistics. By using the results of the research, it will be possible to achieve a competitive advantage for businesses that use them.

Project Title **Work competencies in the context of Industry 4.0 development.**
Coordinator doc. Mgr. Dagmar Cagáňová, PhD.
Start Date 01/01/2019
End Date 31/12/2021
Program VEGA
Annotation Project is aimed at identifying specific new job requirements in form of key work competences and digital skills according to qualification levels defined by the National Qualification Frame of Slovak republic (NQF) in the context of the development of the technological and working environment Industry 4.0. Project is based on an analysis of developments in the field of industry 4.0 development. The aim of the project is to contribute to the actual flow of information between labor market actors, reflecting the development of key competencies and digital skills in practice. The methodological objective of the project is to specify new job requirements according to the qualification levels of the National Qualification Framework in selected production sectors. The project reflects the key challenges in the Industry 4.0 strategy development in Slovak Republic.

Project Title **Identification of priorities for sustainable human resources management with respect to disadvantaged employees in the context of Industry 4.0**
Coordinator prof. Ing. Miloš Čambál, CSc.
Start Date 01/01/2020
End Date 31/12/2023
Program VEGA
Annotation The essence of the scientific project is to analyze the impact of changes in the performance of industrial enterprises on the priorities of sustainable HRM. Management approaches focus mainly on employee and business performance. Changes in the performance of industrial enterprises, related to the digitization increase, the reduction of live work in production, processes improvement, technologies are aimed at organization's efficiency and effectiveness increase. Implementation of new approaches can have an impact on employees of different

generations, while the potential negative effect of these risks is not sufficiently analyzed. The aim of the project is to identify risks in the emergence of new practices, critical impact areas on employees, and explore mechanisms to eliminate these risks. The purpose of the project is to explore the potential of employing disadvantaged groups of employees in the context of changing conditions for enterprises, respecting the uniqueness of different generations of employees.

Project Title	**Network visualization of common and specific elements and documented information of integrated management systems with respect to relevant ISO standards**
Coordinator	doc. Ing. Alena Pauliková, PhD.
Start Date	01/01/2020
End Date	31/12/2022
Program	KEGA
Annotation	The subject of this project is to elaborate a comprehensive overview used on a global scale and subsequent coordination of individual areas of management systems as part of a comprehensive integration for industrial operations including quality management, environment, OSH, energy, information security, transport, corporate social responsibility, business continuity and more. The set of selected areas will include the organization's connections with industrial operations, key customer requirements, leadership, planning, operational support, operations, performance evaluation, and improvement. Co-ordination will be performed using hierarchical organizational diagrams and final visualized by small world networks - Small World Networks and Scale-Free Networks.

PROJECTS OF THE INSTITUTE OF INTEGRATED SAFETY

Project Title	**Implementation of progressive technologies, methods and forms to education in the study branch Safety and Security Science**
Coordinator	doc. Ing. Jozef Martinka, PhD.
Start Date	01/01/2020
End Date	31/12/2022
Program	KEGA
Annotation	The project is aimed at improving the quality of the educational process of students of the 1st and 2nd degree of university study in the study branch Safety and Security Science (Rescue Services) at the Technical University in Zvolen (Fire Protection and Safety Study Programme) and at the Faculty of Materials Science and Technology in Trnava (Integrated Safety Study Programme) based on application of advanced technologies, methods and forms of education. For selected coursed and core thematic areas of the study branch the innovative electronic learning materials and video tutorials will be created, as well as new modern teaching aids using 3D and large-format printing technology. Teaching materials will be prepared for practical exercises based on direct interaction of teacher – student, using modern ICT devices and with Microsoft Education Tools (part of Microsoft Office 365). The level of knowledge will be verified by on-line tests. In addition to creating new multimedia interactive learning materials and improving the competences of

students and graduates, online access and the availability of up-to-date learning materials will also be a benefit for students at other universities and practitioners.

Project Title	**Worldwide unique progressive methods of testing electrical cables for the needs of conformity assessment and verification of the constancy of their parameters as construction products**
Coordinator	doc. Ing. Jozef Martinka, PhD.
Start Date	01/07/2017
End Date	30/06/2021
Program	APVV
Annotation	For most electrical cables within the meaning of Annex V to the Directive of European Parliament and the Council no. 305/2011 on the assessment and verification of constancy of parameters is used system 1+. On 01/07/2017, ends the transitional period and the assessment and verification of constancy of parameters of most electrical cables in the European Union will be carried out only in accordance with EN 50575: 2014. For manufacturers, this will mean the obligation of performing tests of power, control and communication cables for general use in accredited testing laboratories at yearly intervals. Costs for annual testing for one type of cable are in the order of thousands of euros. At a range of several hundred kinds of cables - power, control and communication cables of different diameters, different rated voltage and current load will this obligation mean a heavy financial burden on the production of cables. In the Slovak Republic, production and distribution of electrical cables directly and indirectly employs thousands of workers and represents a significant contribution to GDP. Despite this fact exhibit Slovak cable manufacturer in comparison to the other producers in Europe, but also US and China, low volume of production. For that reason, the costs on annual tests will more significantly share in the price of products. These may significantly jeopardize the competitiveness of Slovak producers in the European Union markets. Even producers in the European Union have in comparison with producers from the US and China low volume of production. Consequences of that fact, and their costs significantly reflected in the price of the product will also threatens their competitiveness. The solution is to develop new innovative tests that will maintain current safety requirements and substantially reduce the cost of testing. The project aims to develop tests satisfying the above conditions.

PROJECTS OF THE INSTITUTE OF APPLIED INFORMATICS, AUTOMATION AND MECHATRONICS

Project Title	**Holistic approach of knowledge discovery from production data in compliance with Industry 4.0 concept**
Coordinator	prof. Ing. Pavol Tanuška, PhD.
Start Date	01/07/2018
End Date	31/12/2021
Program	VEGA

Annotation	The main project goal is creation of a holistic approach of knowledge discovery from production data of heterogeneous control systems in compliance with Industry 4.0 concept. This includes Big Data, Internet of Things, smart sensors, forecasting and decision support methods and tools. The main topic will be proposal of analytic platform to collect, process and analyse big structured and unstructured data sets, utilising Hadoop and NoSQL technologies, for complex process control in production companies. Proposed analytic platform (utilising statistical and inductive learning techniques, e.g. neural networks, fuzzy modeling, decision trees, cluster analysis, etc.) will provide possibilities for gaining new, potentially useful knowledge from data. Subsequently, control strategies will be developed from the gained knowledge using synthesis. Results can be implemented in real-time predictive maintenance and optimization of relevant control paramet.

Project Title	**Using the methods of multi-objective optimization in production processes control**
Coordinator	prof. Ing. Pavel Važan, PhD.
Start Date	01/01/2018
End Date	31/12/2020
Program	VEGA
Annotation	The intention of the project is an exploration of using methods of multi-objective optimization and simulation optimization applied to specific types of production systems. The research will be aimed to the comparison of these methods by the efficiency for acquiring the Pareto set containing the optimal solutions necessary for the production control. The obtained information will be using for the creation of the base of knowledge designated to the qualified support decision in the area of specified production system control problems. The Industry 4.0 strategy supposes the virtual reality and so-called exponential technologies using next to others, where the multi-objective optimization problems belong to. The production process control demands the decisions based on the contradictory goal criteria. It is easier to search the optimal system settings using virtual simulation model of the production system and then to apply them to the real system. The multi-objective simulation optimization could be the answer.

Project Title	**Development of advanced models for design and optimization of heat treatment and joining processes of newly developed high-strength steels**
Coordinator	doc. RNDr. Mária Behúlová, CSc.
Start Date	01/01/2020
End Date	31/12/2023
Program	VEGA
Annotation	The project is focused on the design and preparation of the new types of high-strength steels (AHSS) for automotive industry, including the technologies of their heat treatment and thermo-mechanical treatment, to obtain the optimal combination of specific properties of these materials (weight/strength/elongation). The next step is the investigation of the possibilities of metallurgical joining of newly designed AHSS and the analysis of

development of dissimilar weld joints of AHSS and light-metal alloys (Al, Mg, Ti). The chemical compositions of steels will be proposed using the ThermoCalc software and JMatPro. The influence of technological parameters of heat treatment and material joining processes on the phase composition, microstructure and the final properties of AHSS will be predicted using advanced materials models and simulation models, using which the numerical simulations of investigated processes will be performed in ANSYS, DEFORM and SYSWELD software.

Project Title	**The innovation of the subject Intelligent Control Methods at the Faculty of Materials Science and Technology of Slovak University of Technology**
Coordinator	doc. Ing. Peter Schreiber, CSc.
Start Date	01/01/2018
End Date	31/12/2020
Program	KEGA
Annotation	The project is oriented into the innovation of a subject Intelligent Control Methods (ICM)at the Faculty of Materials Science and Technology of Slovak University of Technology. It is interdisciplinar: it applies intelligent methods into control as well as in the (bio)signals processing. The workplace of applicants owns laboratories with very good technical equipment (controllers, PLCs, different objects of control like production lines, robots, robotized workplaces, segway, ball and plate apparatus, car and helicopter models, helmet for EEG scanning etc.). The relevant software for data acquisition and processing, control and communication in all levels is available too. The laboratories were built as a result of the "University Research Park" project and they are used for research and teaching in the field of traditional control and automation. The goal of the submitted project is to implement intelligent methods and approaches (fuzzy control, optimization by genetic algorithms, identification by neural networks etc.) in more workplaces in those laboratories. New laboratory exercises will be developed and new manuals will be prepared. The subject ICM will be completely innovated. The outputs of the project will be: the innovated subject, new exercises with manuals for more controlled systems, one dissertation and several diploma and bachelor thesis, seminar and projects (1 national, 1 international) submitted with foreign (German) partner.

Project Title	**Extension of the laboratory of mechatronic systems and creation of new study supports**
Coordinator	Ing. Rastislav Ďuriš, PhD.
Start Date	01/01/2018
End Date	31/12/2020
Program	KEGA
Annotation	The ultimate aim of the proposed project is to extend substantialy the present equipment of the „Laboratory of Mechatronical Systems, experimental and diagnostic methods“ by educational, testing and measuring facilities to support the education in subjects such as Mechatronical Systems, Modelling of Mechatronical Systems and Mechanics of Machines and Aggregates supposed to be included in new study program under the accreditation process. The

Laboratory is expected to support the teaching of subjects the course of Experimental Methods and Technical Diagnostics. Improved state of art of the Laboratory should enable to develop the theoretical as well as the practical skills of students learning.in the area of Mechatronics being influenced by innovative educational processes using CAE Technologies, Virtual Instrumentation and E-learning.

Project Title	**Innovation and new learning opportunities in industrial process management with PLC**
Coordinator	Ing. Andrea Némethová, PhD.
Start Date	01/01/2020
End Date	31/12/2022
Program	KEGA
Annotation	The presented project, entitled "Innovation and New Learning Opportunities in Industrial Process Control with PLC", aims to innovate an existing laboratory focused on industrial processes control by PLC. The laboratory currently contains 8 workplaces containing physical models enabling the simulation of selected processes. The aim of this project is to innovate the laboratory to simulate Inovácia a nové možnosti vzdelávania v oblasti riadenia priemyselných procesov pomocou PLC 3/21 Identifikátor: 20190425141260810 the realization of full-fledged workplaces with complex distributed control systems. The aim of this project is to innovate the laboratory so that all workplaces can be fully utilized and even more complex distributed systems can be simulated. This modernized laboratory will also allow the extension of the subject "Programmable Logic Controllers". Another benefit is the possibility of solving bachelor, master and dissertation theses. After implementing new workplaces and elements in the laboratory, this can be used to carry out workshops, create teaching materials and sample enclosures from individual workplaces.

PROJECTS OF THE ADVANCED TECHNOLOGIES RESEARCH INSTITUTE

Project Title	**Time of Flight (ToF) system for Elastic Recoil Detection Analysis (ERDA) based on digital nuclear electronics**
Coordinator	doc. Ing. Maximilián Strémy, PhD.
Start Date	01/01/2018
End Date	31/12/2020
Program	VEGA
Annotation	The ToF ERDA (Time-of-Flight Elastic Recoil Detection Analysis) system will be implemented using the latest digital electronics modules. Extension of the experimental and analytical base of the 6 MV tandem ion accelerator by HE (high energy – tens MeV) HI (heavy ion) ERDA. Determination of the depth concentration profiles of all elements of samples, from hydrogen to atoms with atomic mass of primary ions. The aim of the project is to design and implement the ToF system for the 3D measurement (mass / energy / yield) using the digital nuclear electronics based on high-speed (up to GigaSample/s) digitizers (FPGA).

ToF ERDA solution will be implemented as a real-time control system evaluated as a safety-critical process.

Project title	**Computational design of novel functional materials**
Coordinator	doc. Mgr. Mariana Derzsi, PhD.
Start date	01/01/2019
End date	31/12/2022
Programme	VEGA
Annotation	The project focuses on broadening the vistas of the technologically important systems with transition metals and lanthanides by predicting and targeted design of new as-yet unknown phases using theoretical approaches based on atomic-scale quantum-mechanical modelling, evolutionary algorithms and direct phonon method. The studied systems will encompass new electronic materials for spintronics, multiferroics and superconductors. This study will allow for designing of the most effective and technologically attractive structural forms of the newly predicted phases with metallic elements particularly tuned for the functionality in question in accessible pressure and temperature ranges.

Project title	**Searching for multicomponent character of the flickering in accreting systems**
Coordinator	Mgr. Andrej Dobrotka, PhD.
Start date	01/01/2020
End date	31/12/2022
Programme	VEGA
Annotation	The aim of the project is to study fast stochastic variability generated by mass accretion in cosmic objects, where the main drive mechanism is disc driven accretion, i.e. (for our current focus) cataclysmic interacting binary stars with a white dwarf, X-ray binaries with black holes, or active galactic nuclei with a supermassive black hole in the center. This stochastic flickering do not originate only from one source and has a complicated morphology. The proposed project aims to study the frequency spectrum of variability in order to identify the source. Since all mentioned objects have the same physical process as the main engine, the flickering morphology must also have common features. Our goal is to look for these common features and to create a complex concept of flickering for all objects. For this purpose, we will use high-quality, extensive and multi-frequency data from space missions such as Kepler and XMM-Newton.

Project Title	**Advancement of knowledge in area of advanced metallic materials by use of up-to-date theoretical, experimental, and technological procedures**
Coordinator	prof. Ing. Jozef Janovec, DrSc.
Start Date	01/07/2016
End Date	30/06/2020
Program	APVV
Annotation	The project is focused on the acceleration of progress in gaining knowledge about advanced metallic materials. In the related research the representative part of the Slovak scientific basis will be involved, namely the Slovak University

of Technology (STU) in Bratislava, the Institute of Physics (IP) of the Slovak Academy of Sciences (SAS), and the Institute of Materials Research (IMR) of SAS. To fulfil project tasks, the top-level recently provided equipment will be used, available at the university scientific parks of STU located in Bratislava and Trnava as well as at the scientific centres of SAS located in Bratislava (IP) and Košice (IMR). The experimental research will be combined with calculations from first principles (IP SAS) and thermodynamic predictions (IMR SAS), both the procedures, which the involved researchers reached a world-wide acceptance in. From the thematic point of view, the project implies theoretic and experimental studies of advanced metallic materials mainly related to phase equilibria (new phase diagrams will be proposed and the existing will be refined on), characterization of crystal structures of un- and less-known complex phases, electrochemical and catalytic properties of surfaces, and innovations in production of thin layers, coatings, and ribbons. Expected results will be published in stages in relevant scientific journals, used by the involved researchers in educational process,and consulted eventually with industrial partners to consider the transfer of technological findings in praxis. All the involved institutions have a huge experience with the science promotion and are ready to exert it in the project.

Project title **Noncovalent interactions in systems of increasing complexity**
Coordinator RNDr. Andrej Antušek, PhD.
Start date 01/07/2016
End date 30/06/2020
Programme APVV
Annotation A common idea of this project is providing benchmark wavefunction data (mostly CCSD(T)) that would support DFT predictions of energetics and properties of gradually complex systems. Noncovalent interactions will be analysed, contributions
many-body terms to the non additivity will be evaluated. As a prototype, beryllium clusters will be studied, binding energies per atom of Be_n up to the solid state will be of interest. The focus will be on interactions of biologically relevant amino acid clusters extracted from protein structures in the Protein Data Bank, their geometry and stability. Another class of molecules considered are metal-ligand complexes, including heavy metals. The main goal is to understand the bonding mechanism in context of their size, from small complexes to nanoclusters. Relativistic effects provide one of instruments for this analysis as well as for the analysis of iodine containing species relevant to coolant system of the nuclear reactor and in 12 complexes with antithyroid drugs. Many-body dispersion interactions will be treated using DFT in connection with layered materials and molecular crystals, their structure, elastic and thermal properties and adsorption. The alteration of properties of solute molecules in solvents, is another consequence of intermolecular interactions. This will be considered in relativistic calculations of NMR shielding constants. We combine wavefunction and DFT methods having in mind controlled accuracy. Large systems are treated using DFT, but selection of

functionals is supported by extensive benchmarks on model systems. This will be achieved by further extension of efficiency of the wavefunction methods towards treating model systems closer to large molecules of interest. Important part of the project is the development of relativistic methods as well as improvement of methods for dispersion treatment within DFT. All methodological achievements will be implemented in computer programs MOLCAS, DIRAC and VASP.

Project title **Quest for novel inorganic compounds with nickel, palladium, copper and silver by DFT modelling and ion beam synthesis**
Coordinator doc. Mgr. Mariana Derzsi, PhD.
Start date 01/07/2019
End date 30/06/2023
Programme APVV
Annotation The current project aims at a thorough theoretical and experimental study of all important stoichiometries, which are currently missing from the structure map of binary oxides and halides of Group 10 (Ni, Pd) and 11 (Cu, Ag) metals. Absence of these simple chemical stoichiometries is disturbing and calls for an explanation. What are the reasons for these white spots on the huge seas of chemical stability? Are these compounds truly unstable? Or, maybe, they could be stable but not enough attention was paid to them? Answers to these and related questions will be given within the project using state-of-the-art approaches for search of new materials that will rely on combination of computational modelling at the atomic level and experimental physicochemical techniques, reactive magnetron sputtering deposition and ion implantation. Our strategy meets the urgent need of the modern world for highly effective screening of the unknown potential of available natural resources and the most economic use of available research infrastructures.

Project title **Quantum Monte Carlo for strongly correlated electronic systems**
Coordinator Ing. Matúš Dubecký, PhD.
Start date 01/07/2019
End date 30/06/2023
Programme APVV
Annotation In recent years, single-determinant fixed-node diffusion Monte Carlo (FNDMC) reached high-standard accuracy in a number of diverse systems (where mean-field methods like DFT do not suffice) ranging from weakly bound noncovalent complexes to strongly correlated systems like solid transition-metal oxides at high pressures. Thanks to its favourable CPU cost scaling, parallelism, and direct access to periodicity, FNDMC gains popularity as an unprecedented benchmark tool for large realistic complex many-electron systems. Recent results however suggest, that the expected accuracy is not always accessible, sometimes the results are overvalued, or they depend on the parameters that have been ignored to date. The reason being incomplete understanding of FN approximation (FNA) and its interplay with other possible biases. Our goal is identification and development of deep conceptual understanding of the key FNDMC error sources in strong interaction limit. We plan to uncover the

currently unknown links between generic nodal (position-space) properties (e.g.,topology) of fermionic wave functions, and, their connection to the structure of many-determinant expansions and 1-particle reduced density matrix occupation numbers, as well as separation of electron correlation energy to dynamic and nondynamic (strong, multireference) component, which will enable fundamental understanding of FNA limits and decoupling of FN-bias from other bias sources of FNDMC. We also plan screening of FNDMC accuracy in strongly interacting model systems and unprecedented method developments that go beyond FN approximation. In addition to deep physical insights to the strong correlation effects in complex many-electron systems and limits of FNDMC methodology, the results of the project will enable rational usage and fine bias control of this method valuable for large systems.

Project title **PREPARATION FOR ATHENA MISSION BY ESTABLISHING SLOVAK RESEARCH TEAM ORIENTED TO EXISTING X-RAY MISSIONS AND AGN STUDY**

Coordinator Mgr. Andrej Dobrotka, PhD.
Start date 01/03/2019
End date 28/02/2021
Programme Iný medzinárodný
Annotation The aim of the project is to create and train a new satellite data analysis team, targeting mainly XMM-Newton (ESA), Chandra (NASA) and Swift (NASA) missions aimed at accretion systems, to prepare the currently non-existent platform for the future X-ray mission Athena (ESA). The project aims to have two aspects: X-ray data processing and active galactic nuclei (AGN), the first mentioned having a very weak base in Slovakia, and no longer exists at all, and is one of the main objectives of the planned ATHENA mission. During the first phase, the team must be able to process raw data from XMM-Newton, Chandra and Swift missions to obtain energy spectra and light curves. In the second phase, team will initiate systematic research on AGN and publish its results in scientific journals.

Project title **Towards Realistic Electronic simulations by eXascale quantum Monte Carlo (TREX)**

Coordinator Ing. Matúš Dubecký, PhD.
Start date 01/10/2020
End date 30/09/2023
Programme Iný medzinárodný
Annotation TREX is a highly integrated initiative that gathers most European leading scientists in quantum mechanical simulations of extreme accuracy in the framework of stochastic quantum Monte Carlo methods. This methodology represents one of the highest steps in precision in the ladder of electronic structure approaches and is uniquely positioned to fully exploit the massive parallelism of the upcoming exascale architectures. The marriage of this sophisticated approaches with exascale computing is bound to enable molecular simulations of unprecedented accuracy for complex scientific and industrial applications, meeting the growing demands for robust and predictive calculations in materials design.