

## PROJECTS OF THE INSTITUTE OF MATERIALS SCIENCE

**Project Title** Investigation of the temperature and duration of sub-zero treatment on the microstructure and properties of Cr-V tool steel

Coordinator prof. Ing. Peter Jurči, PhD.

Start Date 01/01/2017

End Date 31/12/2019

Program VEGA

Annotation The main goal of the project is to determine the optimal temperature and duration of sub-zero treatment with particular interest to get the best complex of microstructure and important properties of Cr-V ledeburitic steels. The second object of the interest is to determine a "window of properties improvement" e.g. the combination of sub-zero treatment and tempering temperatures where simultaneous improvement in strength and toughness can be achieved. A commercially available PM Cr-V ledeburitic tool steel will be used as experimental material. The effects of heat treatment variables such as the temperature and the duration of sub-zero treatment and tempering regimes, at constant regimes of the austenitizing and quenching, on such important characteristics like the microstructure, hardness, toughness, fracture toughness and wear resistance will be investigated. In the project, variety of investigation techniques will be utilized complementarily, which makes it possible to achieve the main goal of the project.

**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** Diagnostics of special glasses with optimized ionic conductivity

Coordinator Mgr. Ondrej Bošák, PhD.

Start Date 01/01/2017

End Date 31/12/2019

Program VEGA

**Annotation** The project is orientated on study of structure and physical properties of a new special glasses systems based on chalcogenides and heavy metals oxides with a higher content of ionic bonds or higher concentration of alkali ions respectively. These special glasses will be designed for optoelectronic applications. There is possibly using these materials for solid electrolytes. From the professional point of view it is the study of changes in the glass structure generated by the change of chemical composition, investigation of the preparation technology and effect of increased temperature and humidity. Changes in structure usually affect formation of a new phases, which can be monitored using electrical and optical methods. The aim of the project is a detailed description of the structure and properties of glasses enhanced by the results of the analysis of electrical and dielectric parameters.

**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 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 chalcogenides 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: Research of the coating/ substrate interphase modification to increase hard coating adhesion**

Coordinator: prof. Ing. Ľubomír Čaplovič, PhD.

Start date: 01/07/2016

End date: 30/06/2019

Programme: APVV

Annotation: In the last decade, hard coatings based on nitrides or carbonitrides of transition metals play significant role in increasing the lifetime of the cutting and forming tools, but also in specific products of mobile devices. The main requirement for this type of material is high hardness and abrasion resistance. However, in the case of dynamic loading and frequent alternation of heat cycles, the adhesion of the coating to the substrate is the decisive factor. The object is just focused to this area with the main aim to find and optimize physical processes to enhance the adhesion ability of selected types of coatings and create a mathematical model that could describe the physical processes involved. The specific goal is to verify the influence of the initial state of the substrate surface prior to the coatings deposition both in terms of structural, thermal and deformation characteristics of the coating/substrate phase interface. Different methods for cleaning of substrates, surface preparation and deposition technologies will be utilized for these tasks. The techniques of plasma, magnetron and ion sputtering as well as cathodic arc evaporation will be mainly used. The experimental methods such as electron microscopy, X-ray diffraction analysis, Auger electron spectroscopy and optical emission spectroscopy as well as a special ion beam/matter interaction based techniques (RBS, PIXE) will be utilized for the study and explanation of processes that could occur at the coating/ substrate phase interface. The method of FEM will be used for the clarification of effects of both internal and residual stresses to the coating/ substrate interface character. The output will be a comprehensive analysis of the influence of individual parameters of used processes on increasing of interface adhesion and drafting the proposals for their applications in the preparation of hard coatings with enhanced exploitative properties.

**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 FeCu<sub>1.8</sub>C<sub>0.7</sub> and FeMo<sub>0.5</sub>Ni<sub>0.5</sub>C<sub>0.6</sub>) is its density in range 6.9 -7.1 g.cm<sup>-3</sup>. 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  $> 7.4 \text{ g.cm}^{-3}$  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: 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** Research of new alloys for direct soldering of metallic and ceramic materials  
**Coordinator** prof. Ing. Roman Koleňák, PhD.  
**Start Date** 01/01/2017  
**End Date** 31/12/2019  
**Program** VEGA  
**Annotation** The project is oriented to fundamental research of new alloys for direct soldering of metallic and ceramic materials. The research of soldering alloys Sn-Ti, Sn-La, and Sn-In is mainly concerned. The new soldering alloys will be prepared experimentally by alloying with small amounts of active elements (Ti, In, La and several other elements from the group of lanthanides). The solders will be designed with the aim to be applicable for direct soldering with utilisation of laser and power ultrasound technologies. The tests of technological solderability of ceramic and metallic materials will be performed by use of the new soldering alloys. The structural character of solders and soldered joints will be determined at different soldering conditions. Also the interactions of soldering alloys type Sn-Ti, Sn-La and Sn-In with the surface of ceramic materials will be studied. The individual mechanisms of joint formation from the viewpoint of its strength, formation speed, life etc. will be compared.

**Project Title** Research of deformation processes using spatial reconstruction of microstructure and shape of formed parts  
**Coordinator** prof. Ing. Maroš Martinkovič, PhD.  
**Start Date** 01/01/2016  
**End Date** 31/12/2019  
**Program** VEGA  
**Annotation** Final properties of forming metal parts are affected by production technological processes. Due to forming not only shape of body is changing, but so as structure anisotropy is increased-- grain boundaries orientation in various places of piece. Research, development and application of stereology methods of statistic reconstruction of three-dimensional plastic deformed metal material structure in examining the dimensional changes forming body using industrial computed tomography and coordinate measuring machine. Utilization of this results to a detailed lead analysis of material structure changes, resulting properties and consequential technological processes optimization and knowing quantitative dependences "technological parameters - microstructure -- properties".

**Project Title** The study of physical and mechanical properties, mechanability and surface treatment of Ti and YTi composites prepared by powder metallurgy  
**Coordinator** prof. Ing. Peter Šugár, PhD.  
**Start Date** 01/01/2017  
**End Date** 31/12/2019  
**Program** VEGA

**Annotation** In the years 2013 - 2015 has been optimized powder metallurgical technology of preparation of Ti samples with respect to the resulting mechanical properties of the material. The following low-temperature methods of densification were used: forging and direct hot extrusion. The acquired knowledge allowed us to develop, prepare and patent composite materials for biomedical applications Ti-Mg. Now, the technology makes it possible to prepare Ti composites which cannot be prepared by high temperature methods, since the embedded phase reacts with the Ti matrix. The goal of the project is the preparation of composites with not reacted embedded phase and research of their physical and mechanical properties. Consequently, it is necessary to examine machine ability and surface treatments of such materials for potential industrial applications. The resulting goal is to prepare Ti-based matrix composite lighter than Ti with improved surface properties.

**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 joints 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 prepared 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 difficult-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 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 from 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 professional 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 project 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** **Research on welding of progressive light alloys by beam welding methods**

Coordinator prof. Ing. Milan Marônek, CSc.

Start date 01/07/2016

End date 31/12/2019

Programme: APVV

Annotation: The major objective of the project is to bring a new knowledge in the field of welding Ti and Al-Li alloys by laser and electron beam welding methods. These advanced alloys have perspective of their further exploitation also in other industrial areas, where weight reduction and corrosion resistance is required. Nowadays, beam welding methods are used in mass production even more frequently, because of their high productivity and minimal degradation effects on welded materials. However, the knowledge about beam welding of these alloys significantly absents. The weldability of Ti and Al-Li alloys, the structural analysis and the tests of mechanical properties will be investigated in particular stages of the project. Special focus will be devoted to find the correlation between the dominant technological parameters of the process and properties of performed weld joints. The modern technological equipment and advanced methods of weld joints analysis will be used. The research team has sufficient experience in this research field and adequate potential to accomplish defined objectives. The project has the ambition to push the knowledge boundaries of the welding process of selected Ti and Al-Li alloys by laser and electron beam welding.

**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 identification 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 production 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.

## **PROJECTS OF THE INSTITUTE OF INDUSTRIAL ENGINEERING AND MANAGEMENT**

**Project Title** **The impact of the coexistence of different generations of employees on the sustainable performance of organisations**

Coordinator prof. Ing. Miloš Čambál, CSc.

Start Date 01/01/2017

End Date 31/12/2019

Program VEGA  
Annotation Essence of the presented scientific project is exploring impact of existence and interactions of employees generations found in organizations, their and organization performance. At the end of the 2nd decade of 21st c. after arrival of generation Z on labour market'll be organizations comprised of 5 generations with vastly different characteristics. Interaction of these can act negatively on processes that occur in organizations. These processes've a significant impact on reduction of their performance and competitiveness. On the other hand, however, create potential for improving their performance. This's reason why project focused on identification and analysis of key aspects of different employees generations and to assess impact on performance of employees and entire organization. The project goal's to examine potential positive interactions between various employees generations and use of potential to achieve sustainable performance of organisations in terms of multigenerational communities.

**Project Title System identification of complex preconditions for supporting innovation and employment in the less developed regions of Slovakia**

Coordinator doc. Ing. Marek Jemala, PhD.

Start Date 01/01/2017

End Date 31/12/2019

Program VEGA

Annotation This project of GOAL-ORIENTED BASIC RESEARCH has the main goal systematically to identify more complex preconditions, general conditions, specifications, core processes, key issues and risks, but also the benefits and competencies necessary for the development of industrial innovation and the support for higher employment in less developed regions of Slovakia. With the orientation to more environmentally, socially and culturally sustainable ways of manufacturing and doing business. This research will be mainly based on verification and possible improvement of the management and innovation assessment methodology of the University of Cambridge as well as the innovation assessment methodology already applied in Lower Austria (I-AM Lower Austria). The focus of this research will be mainly on systemic analysis, comparison, assessment and categorization of research, innovation, technology, manufacturing, human, financial and associated institutional processes, their determinants in the surveyed companies/regions.

**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 E-platform for Improving Collaboration among Universities and Industrial Enterprises in the Area of Education**

Coordinator doc. Mgr. Dagmar Cagáňová, PhD.

Start Date 01/01/2018

End Date 31/12/2019

Program KEGA

Annotation The aim of the project is to design and implement a portal solution based on Internet services, which will allow to improve the connection between education process at universities and the requirements of industrial practice. This connection can be made at several levels such as assignment and management of final and technical thesis topics, project preparation within and across subjects, internships, practice or field trips. At the moment the communication between industry and universities in these areas is conducted by two parallel two-way information channels, between university and industry and also students and industry. The current academic information systems used at STU in Bratislava, Technical University in Zvolen, Slovak agricultural University in Nitra, Pan European University in Bratislava and Constantine the Philosopher University in Nitra, developed at Mendel University in Brno, does not allow direct communication between the university - industry - students . In addition to limited communication the AIS does not contain modules to support the proposal process and control of final thesis topics (as the same topics can only be addressed with a minimum interval of three years), into which all three subjects would directly enter. Linking public portal with the existing AIS would contribute to simplifying and improving administrative processes, enhancing the theses to be of higher quality and up to date, simplifying originality check process, proposing and executing of topics directly linked to business practice, the choice of student by an enterprise on the basis of his/her study results and recommendations, which will ultimately have a positive impact on the graduates success. An indirect benefit of the project will be the reduction of information inequality between businesses and universities.

**Project Title Cultural Opening- diversity and intercultural competences in the context of the refugee crisis**

Coordinator doc. Mgr. Dagmar Cagáňová, PhD.

Start Date 01/07/2017

End Date 01/07/2019

Program BMBF Funds - Bundesministerium fur Bildung und Forschung

**Annotation** A multilateral collaboration between Germany, the Czech Republic, Latvia, Serbia, Hungary and Slovakia aims at drafting a mutual Horizon 2020 proposal as well as intensifying the collaboration between the European partners named above to build a network for mutual research and knowledge transfer. A long-term and if possible permanent collaboration for the H2020 project and probably other follow-up projects as well as knowledge transfer for science and society are to be pursued. The network focusses on the strengthening of internationalisation, Europe-orientation, and competitiveness of institutions in research and education and furthering an innovation union.

**Project Title** **Automotive JUNIOR academy**

**Coordinator** doc. Mgr. Dagmar Cagáňová, PhD.

**Start Date** 23/06/2016

**End Date** 15/11/2019

**Program** Iný domáci - vzdelávací

**Annotation** AJA was created as a joint project of the Automotive Industry Association of Slovakia, Volkswagen Slovakia, PSa Groupe Slovakia, Kia Motors Slovakia and slovak universities, Žilina University in Žilina, STU Faculty of Mechanical Engineering in Bratislava and STU Faculty of Materials Science and Technology in Trnava. AJA is a summer thematic academy organized in Trnava, Žilina and Bratislava and is intended for children of the 7th and 8th grades of elementary schools of for students of tercia, resp. quarta at eight-year grammar schools.

**Project Title** Enhance skills and competences to boost material innovations and eco innovations in automotive industry

**Coordinator** doc. Mgr. Dagmar Cagáňová, PhD.

**Start Date** 01/01/2018

**End Date** 31/12/2019

**Program** Interreg – Danube Transnational Programme (DTP)

**Annotation** The main project aims to address the shortage of knowledge caused by the lack of highly qualified and competent experts in the field of new materials research and reuse of hard recyclable materials in and out of the automotive industry through the implementation of dual learning elements and joint research centers. The project will result in the improvement of educational programs and research fields, focusing mainly on the implementation of dual education and increasing competences in the field of research management and cooperation.

## PROJECTS OF THE INSTITUTE OF INTEGRATED SAFETY

**Project Title** Educational Centre for Integrated Safety

Coordinator doc. Ing. Jozef Martinka, PhD.

Start Date 01/01/2017

End Date 31/12/2019

Program KEGA

Annotation The aim of the project is the creation of a joint workspace of three Slovak universities devoted to lifelong learning of experts in the field of integrated safety. The main benefit of the project is to facilitate the application of fresh university graduates in the labor market.

**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** **Design, analysis and optimization of processes of metallurgical joining for progressive materials using numerical simulation**

Coordinator doc. RNDR. Mária Behúlová, CSc.

Start Date 01/01/2016

End Date 31/12/2019

Program VEGA

Annotation The project is focused on the design, numerical simulation, experimental verification and scientific explanation of the possibilities of joining the advanced light alloys based on Al, Mg, Ti, as well as new generations of high strength steels and their combinations including the formation of weld joints of these materials with composites/plastics. The preparation of sound welds is supposed using concentrated energy sources, welding methods in solid state, special, modified and hybrid welding methods, soldering and mechanical joining.

**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 interdisciplinary: 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 substantially 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-

**Project Title V4+ Academic Research Consortium integrating databases, robotics and languages technologie**

Coordinator Ing. Štefan Svetský, PhD.  
Start Date 01/06/2018  
End Date 30/09/2019  
Program International Visegrad Fund - Strategic grants  
Annotation The proposed sustainable V4+ Academic Research Consortium will tackle regional problems related to EU ICT research priorities in several issues: Partner search for Horizon 2020, building of the digital platforms of the future, language barriers, technology-enhanced learning, scientific cultural heritage, know-how exchange (there is ca 30 ICT calls for Horizon 2018-2020). The focus will be on networking of the V4+ partners in order to integrate their research expertise, perform Partner search and benchmark these issues by using the virtual technological platform. Horizon 2020 covers these strategic priorities and has a specific funding instrument available for bridging research teams: Coordination and Support Actions, including Partner search projects. Such support does not exist in Slovakia, even with institutional academic grants. This is barrier for participation of researchers in Horizon or for acting in V4 regional cooperation for competitiveness and connectivity. It is important that V4 grants enable such support. Solving the above mentioned issues requires joined research expertizes with in EU consortia. So to create compatible V4 consortia for preparing research subjects for Horizon is strategic, also due to the bad situation regarding under-use of EU competitive research funds in all V4+ countries. The idea of Educational Virtual Robot <http://www.ideal-ist.eu/ps-sk-99947> started collaboration of partners. They found that by joining their expertizes (databases, robotics and languages technologies) they could participated in Horizon as V4+ Consortium.

## 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** **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<sub>n</sub> 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 (FN-DMC) 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, FN-DMC 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** **Predictive modelling of new functional materials for technological applications**

Coordinator doc. Ing. Maximilián Strémy, PhD.

Start date 01/04/2018

End date 30/09/2019

Programme Schéma Návraty

Annotation The project focuses on search for novel materials for innovative technologies by means of atomic-scale computational modelling. We will gain new insights into fictionalization of transition metals in form of new inorganic compounds and their attractive solid-state phases. The computational approach will be based on learning algorithms combined with quantum-mechanical Density Functional Theory methods. The project will be realized in two stages. In the first stage, new systems with transition metals will be mapped and their crystal

structures characterized. In the second stage, we will shift our attention to physico-chemical properties with the aim to functionalize the new systems for applications in electronics and spintronics.

<b>Project title</b>	<b>STU ako líder Digitálnej koalície</b>
Coordinator	Dr.h.c. prof. Dr. Ing. Oliver Moravčík
Start date	01/01/2019
End date	31/12/2019
Annotation	<p>Within the project, the Slovak University of Technology in Bratislava focuses on fulfilling the commitments arising from its membership in the Digital Coalition as one of its main initiators in the following areas:</p> <p>Innovate education in computer science programs, list socially current and attractive topics of team, semester and year projects, final, diploma, dissertation thesis according to internationally recognized standards, Develop ICT talents at the university, encourage student participation in international competitions, mentor and financial support of young researchers; Conduct research in promising areas of ICT, including areas such as web-oriented technologies, cyber security, Big Data, Cloud Computing, artificial intelligence, etc.</p> <p>Prepare and present a long-term strategic research project in the industrial technologies for the 21st century, exploiting the synergy of progressive materials research and digital technologies (including Industry 4.0). The project focuses mainly on meeting the strategic objectives within the area of Human Resources, namely achieving consistency between motivation of employees and institutional funding for employees working in areas directly related to STU commitments in the digital coalition, where the difference in financial valuation outside the academic environment is significantly higher . This will increase the motivation of the investigators and at the same time we will strengthen the human resources when the project investigators are rewarded based on the achieved results of the project. Indirectly but significantly, the project intervenes in the field of education and research and creative activities, as it will improve the quality of study programs, promote quality research results and also attract talented young people to study and work at STU.</p>