PROJECTS OF THE INSTITUTE OF MATERIALS SCIENCE

Project Title	**Corrosion stability of advanced zinc, aluminium and tin alloys**
Coordinator	Mgr. Marián Palcut, PhD.
Start Date	01/01/2014
End Date	31/12/2017
Program	VEGA
Annotation	The goal of this project is to investigate the corrosion stability of phases in Zn, Al and Sn alloys. The studied materials can be used, for example, as light materials for automotive and aviation industries, steel protection coatings or lead-free solders for microelectronics. The alloys shall be prepared by a controlled melting of pure elements. The corrosion resistance will be studied in aqueous electrolytes. Moreover, the alloys stability shall be investigated in simulated off-shore conditions by a salt spray test. Selected samples will undergo a high temperature oxidation testing in corrosive atmospheres. Furthermore, mechanical properties will be investigated and a stress corrosion cracking behaviour shall be characterized. The oxidation products will be studied by a combination of methods, including X-ray diffraction, energy dispersive spectroscopy, transmission electron microscopy and infrared spectroscopy. The aim of the project is to identify corrosion resistant alloys for practical applications

Project Title	**Application of complex thermal analysis and computational thermodynamics at investigation of processes in advanced materials systems**
Coordinator	doc. Ing. Roman Čička, PhD.
Start Date	01/01/2014
End Date	31/12/2017
Program	VEGA
Annotation	The project is focused on application of experimental and computational thermodynamics at the investigation of processes and phase equilibria in selected materials systems as complex metallic alloys, advanced tool steels, austenitic stainless steels, hardenable aluminium alloys and lead-free solders. In experimental part the complex thermal analysis of investigated systems will be performed, together with the measurement of some important thermophysical properties and analysis of structure. In computational part the phase quilibria and processes occuring in the investigated materials during controlled temperature programme will be modeled using Thermo-Calc, JMatPro, Dictra, ANSYS, SYSWELD, DEFORM and MATLAB software. The aim of the project is to improve the prediction of phase equilibria and processes in materials systems, using advanced techniques of computational thermodynamics.

Project Title	**Preparation and characterization of the properties of new types of hard coatings for tool materials**
Coordinator	prof. Ing. Ľubomír Čaplovič, PhD.
Start Date	01/01/2015
End Date	31/12/2018
Program	VEGA
Annotation	The submitted project is aimed on development of new type superhard coatings for tool materials with enhanced useful properties. The project is based on gathered knowledge about correlation of structural and stress relations in hard and superhard nitride coatings of transition metals in monolayer or multilayer system on in advanced prepared surface of substrate which is basically tool steel or cemented carbide. By application of two technological processes of creating functional coatings (cathodic arc evaporation and magnetron sputtering),deposition process and its effects of doping of additional interstitial elements (boron, carbon) will be analyzed as well as substitutional elements such as aluminium and silicon in order to achieve a nanocomposite morphology of these coatings.

Project Title	**Preparation and characterization TiC nanocomposite coatings by HiPIMS method for automotive applications**
Coordinator	prof. Ing. Ján Lokaj, CSc.
Start Date	01/01/2015
End Date	31/12/2017
Program	VEGA
Annotation	This project focuses on the investigation of plasma parameters and the deposition behaviour of HiPIMS process with pre-ionization. Thus, the aim of this project is to perform diagnostics of the plasma generated by powerful pulses with pre-ionization in order to understand the relationship between the process parameters and local parameters of deposition plasma, which actually govern plasma processes and plasma-surface interaction. The aim of this project is also to prepare and characterize nanocomposite TiC wear-resistant coatings targeted for automotive applications where high load-bearing capacity and thermal stability, low friction, and wear resistance are the primary requirements.

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 thechange 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: **Analysis of structural changes and characterization of electric properties of special glasses designed for optoelectronic applications**

Coordinator: doc. Ing. Mária Dománková, PhD.

Start date: 01/01/2016

End date: 31/12/2017

Programme: APVV

Annotation: The project is orientated on the support of cooperation between Slovak and French partners in the field of 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. 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 project will provide extension of the cooperation at preparation of common outputs and publications oriented on diagnosing of special glasses designed for optoelectronic applications, possibly for solid electrolytes. 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: **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 leading 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 coatingsubstrate phase interface. Different methods for cleaning of substrates, surface exposition 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	**Physical properties of glasses designed for applications in infrared region of spectrum and memory devices**
Coordinator	prof. Ing. Marian Kubliha, PhD.
Start Date	01/01/2017
End Date	31/12/2018
Program	APVV
Annotation	The proposed project aims to support co-operation between Slovak, Czech and Serbian partners in the area of preparation of special glasses and investigation of their physical properties in view of their possible applications in infrared region of spectrum or as memory devices. From the scientific point of view the project will study the relationship between structural changes in glasses and their physical properties. These structural changes are usually manifested by the creation of new phases, that can be observed by various techniques. We will pursue particularly structural changes manifested in optical and electrical properties of investigated glasses. The project will contribute to the investigation of the nature of processes in non-crystalline structures by means of selected experimental techniques such as transmission and photoluminescence spectroscopy, dielectric (impedance) spectroscopy and thermo-kinetic analyses etc. The aim of the project is searching for correlations between physical properties of investigated glasses obtained experimentally and designing models for description of processes in non-crystalline structures.

Project Title	**Investigation of design and manufacturing methods for coils from round high-temperature superconducting conductor**
Coordinator	Dr.-Ing. Marcela Pekarčíková
Start Date	01/07/2015
End Date	31/12/2018
Program	APVV
Annotation	Investigation of methods for design and manufacturing of superconducting magnet coils from high temperature superconducting tapes using an original conductor architecture and innovative cooling concept is in the core of the proposed project. Superconducting tapes, laid helicoidally on metallic tube with diameter between 3 and 8 mm, form the cable conductor that can be cooled by the flow of coolant (liquid nitrogen, He gas) through the tube. Thermal insulation of the coil wound from such conductor can be very simple from the low cost polyurethane foam without necessity of vacuum. Because the properties of superconductor depend on temperature, magnetic field and mechanical strain, optimization of the conductor architecture and of the manufacturing process requires extensive modelling aimed at solving

mechanical, electromagnetic and mechanical problems. Essential properties of used materials will be determined by experiments employing specialized measurement techniques and structural investigation methods. Higher level of problem complexity is expected in the design and manufacturing of a coil utilizing the optimally designed conductor. Final test of the proposed concept will be carried out on the coil of 120 mm inner diameter hosting in 4 layers 80 turns of conductor able to carry at least 1000 A when cooled by a liquid nitrogen flow, with thermal insulation less than 20 mm thick.

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: **Research and develoment of advanced materials, processing and automation technologies for direct manufacturing and application**

Coordinator: doc. Ing. Martin Kusý, PhD.

Start date: 01/09/2011

End date: 31/08/2018
Programme: NV Bekaert SA
Annotation: The subject of the research will be Research of advanced materials, processing and automation technologies for direct manufacturing and application. The aim of the project is to bridge basic and applied research in the field of advanced materials with application and manufacturing leading to competitiveness and sustainable growth of both partners. A valuable and unique aspect of the research project is broad involvement of students of master and doctoral degree in up-to-date research activities.

Project title: Contract on the Lump Sum related to the Visegrad/ V4EaP Scholarship forKrzysztof Labisz 51601052 concluded for study/ research project
Coordinator: doc. Ing. Martin Kusý, PhD.
Start Date 01/09/2016
End Date 31/07/2017
Program Visegrad/V4EaP Scholarship 51601052
Annotation The project was realized in laboratories of UMAT MTF STU in Trnava. The aim of the study was to characterize the microstructure of Al alloy in a state after extensive plastic deformation and surface remelting.

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 influence of selected characteristics of machining process on achieved quality of machined surface and problem free assembly using high Technologies.**
Coordinator	doc. Ing. Peter Pokorný, PhD.
Start Date	01/01/2014
End Date	31/12/2017
Program	VEGA
Annotation	The project is focused on research of selected characteristics of machining process (cutting forces, thin walled parts machining, tool wear and tool renewing, cutting fluids and machining strategies). Characteristics of machining process affect the quality of achieved surface. The project uses high Technologies, which are situated in centre of excellence of 5 axis machinig (high speed milling machine tools, ultrasonic milling tool, laser milling tool, tool grinder). On the geometric and dimensional accuracy depends the condition of assembly or more precise, the result of assembly process. Therefore the methodology will be designed in order to adjust machining technology with demands of geometric specification of parts.

Project Title	**Establishing the patterns of the structure and properties formation in high-speed steels during melting and casting in vacuum**
Coordinator	prof. Ing. Alexander Čaus, DrSc.
Start Date	01/01/2015
End Date	31/12/2018
Program	VEGA
Annotation	With proper choice of an appropriate nomenclature the durability of cast cutting tools (CCT) can be better than that of conventional tools. However, for successful application of CCT it is necessary to provide adequate impact toughness of cast high speed steel (HSS). From this point of view casting into metal moulds is more attractive because due to high rate of solidification this technology provides enhanced alloy density, fine-grained cast structure, consequently enhanced mechanical properties, primarily impact toughness. Disadvantage is the low life of moulds when casting HSS.

Project Title	**Research of laser surface texturing and its application in the sheet metal forming processes tribological conditions optimization**
Coordinator	prof. Ing. Peter Šugár, PhD.
Start Date	01/01/2015
End Date	31/12/2018
Program	VEGA
Annotation	The project is aimed at the research of the laser texuring of metal spinning tools. Two fields of interest are solved in this project. The goal is optimization of rolling friction conditions in the contact area spinning tool -- formed part with minimal quantity of lubricants and creation of assumptions for improvement of the spun part surface quality while reducing the intensity of tool wear and unwanted adhesion sticks formation.

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 detailedlead 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, CSc.
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	**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	**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	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	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	**Research and development of a new autontomous systom for checking a trajectory of a robot**
Coordinator	Dr.h.c. prof. Ing. Pavol Božek, CSc..
Start Date	01/01/2015
End Date	31/12/2017
Program	VEGA
Annotation	The research project deals with implementation of hybrid sensors - an Inertial Navigation System which will be utilized for the calibration of a robotic workplace. The calibration is necessary for adapting the simulation of a production device model to real geometric conditions. Constructing the model of the production device, as well as creating the corresponding programmes of robots by means of a simulation system represents an exact picture of reality. The deflections of reality from the simulation arise from different reasons (position of work piece,geometric accuracy of a tool, etc.). The proposed INS will be utilized for their calibration without using the calibration agents. It will lead towards great simplification of calibration in practice.

Project Title	**University textbook "The means of automated production" by interactive multimedia format for STU Bratislava and Kosice**
Coordinator	Dr.h.c. prof. Ing. Pavol Božek, CSc.
Start Date	01/01/2015
End Date	31/12/2017
Program	KEGA

Annotation The submitted project proposal is oriented on creating and integration of the content and design of multimedia applications to support the teaching of the newly accreditted subject Means of automated production via written and interactive multimedia form to continuously complement and improve the level of technical subjects related to automation and their control systems at universities. The support of a better, stronger, more efficient perception of information from the textbooks in the subject "Means of automated production" (texts, images, graphics, speech, animations, video sequences) is enabled by multimedia and are presented in several formats.

Project title: Research of new soldering alloys for fluxless soldering with application of beam technologies and ultrasound

Coordinator: prof. Ing. Roman Koleňák, PhD.
Start date: 01/10/2013
End date: 31/05/2017
Programme: APVV
Annotation: The project is oriented toward the research of environmentally friendly solder alloys and conditions of soldering with progressive technologies. The designed and experimentally manufactured solders will be used for soldering of metallic and ceramic materials at higher application temperatures. For assuring the wettability of ceramic and hard-to-solder materials, the solders will be alloyed with active elements and the metals from the group of lanthanides. The tests of technological solderability of ceramic and metallic materials will be performed by use of new soldering alloys at flux-free soldering, with application of laser technologies, power ultrasound and electron beam. The structural charakteristics of solders and soldered joins will be studied at different soldering conditions.

Project title: Development of new multicomponent environmentally- friendly lead-free solder for low-cost electronic assembly

Coordinator: doc. Ing. Erika Hodúlová, PhD.
Start date: 01/01/2016
End date: 31/12/2017
Programme: APVV
Annotation: The project aims at developing and manufacturing complex multiphase materials free of toxic elements content, with enhanced mechanical properties and moderate costs compared to commonly used zero-Pb solder alloys. Preference is given to metal matrix composites, Sn-, Cuand Ag-based alloy systems with the small addition of In and Bi. Implementation is focused on sustainability, where an environmental advantage will be leveraged through the utilization of cheap, non-toxic raw materials by advanced recovery methods. To date, the most widespread Pb-free replacements for lead-bearing solders are binary alloy systems for high-temp service environments Sn-Ag-Cu baseline alloys, the application of which poses a number of technical problems. Inferior tensile behaviour, poor creep resistance, low conductivity and high

melting temperature mostly yields narrow process window, soldering failures and weak life cycle performance. Cost aspect and the compensatory addition of critical elements are the prime challenges to face.

Project title: **Challenges in joining of titanium alloys**
Coordinator: doc. Ing. Erika Hodúlová, PhD.
Start date: 01/01/2016
End date: 31/12/2017
Programme: APVV
Annotation: Joing is literally where all parts of the manufacturing process come together, and thus joing processes are essential to virtually any manufactured product. In particular, joing of titanium alloys is of paramount importance for the aeronautic, aerospace, automobile and biomedical industries. Accordingly, the main objective of the project under proposal is to develop new strategies to join Ti alloys to themselves and to other alloys. Similar and dissimilar joints will be processed by fluxless soldering using beam technologies and power ultrasound. Reactive multilayers will be used to enhance the joining process. These multilayers will act as highly localizated heat sources. The advantage of using reactive multilayers as filler material will be evaluated. The joints processed will be (micro)structurally and mechanically characterized in order to identify for each case the most adequate joining process and the most promising filler materials.

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.

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:	**Innovative methods of sheet metal forming tools surfaces improvement - R&D**
Coordinator:	prof. Ing. Peter Šugár, PhD.
Start date:	2015
End date:	2017
Programme:	FormTool MANUNET-2014-11283

Annotation: The project is focused on developement and verifying a new advanced technology of sheet-metal forming tools surfaces improvement in order to obtain better performances, lower costs and lower environmental impacts of sheet-metal parts production processes. The attention is paid to issue of stamping and metal spinning forming of weld joints. Special focus will be devoted to finding the correlation between the crucial technological parameters of the process and properties of performed weld joint. The project has the ambition to push the knowledge boundaries of the welding process of selected duplex stainless steels by the concentrated energy sources, such as laser and electron beam.

Project Title **Research of electron beam complex generation designed to vacuum welding of aluminum and magnesium alloys**
Coordinator prof. Ing. Koloman Ulrich, PhD.
Start Date 01/07/2015
End Date 30/06/2018
Program STIMULY Req-00048-0005
Annotation The strategic objective of the industrial (applied) research and experimental development project is an overall increase of technical parameters the critical modules of electron beam welding technology complexes comparable to world level.

PROJECTS OF THE INSTITUTE OF INDUSTRIAL ENGINEERING AND MANAGEMENT

Project Title **The Model of the implementation of controlling as a management tool within medium enterprises in the engineering and electronics industries**
Coordinator prof. Ing. Dušan Baran, PhD.
Start Date 01/01/2016
End Date 31/12/2018
Program VEGA
Annotation The research project deals with the current and very important problems of the research and application of advanced control methods in terms of economic sciences. The project analyses the current state of implementation of modern management methods in Slovakia and abroad, especially in the EU and the U.S., with a focus on medium-sized enterprises. The project assesses the internal and external conditions that implementation. Formulates the basis for the creation of scientific foundations subsystem and controlling instruments (subject, basic concepts, explanations and definitions examination). Based on this analysis project defines and develops the already used methods , tools , resources , forms , models and management techniques in the conditions of market economy . At the same time project proposes a unified model subsystem

implementation and controlling instruments in the business community, focusing on a group of medium-sized enterprises.

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 emploees 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	**An innovative approach to legislative coordination of environmental protection through the visualization on the basis of the phenomenom Small World Networks**
Coordinator	doc. Ing. Alena Pauliková, PhD.
Start Date	01/01/2015
End Date	31/12/2017
Program	KEGA
Annotation	The purpose of this project is to develop a comprehensive review and subsequent coordination of environmental legislation as part of a system of ambient protection. Selected set of laws which form part of the environmental legislation will include laws, regulations, decress, international treaties and agreements and other relevant provisions of the national character. Coordination will be done using hierarchical organizational charts and finally visualized usin Small World Networks.

Project Title	**INNOVAT:Social Innovation for Youth participation. Entre-& Intrapreneurship education to foster business-oriented thinking**
Coordinator	doc. Mgr. Dagmar Cagáňová, PhD.
Start Date	01/01/2016
End Date	31/12/2017
Program	ERASMUS+
Annotation	InnovaT wants to strengthen the capabilities of 7 social organisations that work in the field of youth: 4 from Europe (Spain, Portugal, Greece and Romania) and three from Latinamerica (Nicaragua, Colombia and El Salvador) in order to improve their work in the YOUTH PARTICIPATION SECTOR and specifically working in 3 KNOWLEDGE AREAS: Methodologies for social innovation ICTs tools Social entrepreneurship and communitarian development This project wants to contribute in the implementation of "Europe 2020" strategy, working specifically in the fights against poverty and social exclusion of youth.

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	**Creative Europe: Innovative methodologies for Young Social Enterpreneuship**
Coordinator	doc. Mgr. Dagmar Cagáňová, PhD.
Start Date	01/01/2016
End Date	31/12/2018
Program	ERASMUS+
Annotation	

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 Mechanicla 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 8thgrades of elementary schools of for students of tercia, resp. quarta at eight-year grammar schools.

PROJECTS OF THE INSTITUTE OF INTEGRATED SAFETY

Project Title	**Studying the use of advance oxidative processes for metalworking fluids lifetime extension and for their following acceleration of biological disposal at the end of the life cycle**
Coordinator	prof. Ing. Maroš Soldán, PhD.
Start Date	01/01/2014
End Date	31/12/2017
Program	VEGA
Annotation	Project follows the possibility of using low concentrations of O3 as a progressive method of hygienisation of MWFs during the period of their use in machining. It is for the purpose of extending the lifetime of MWFs, protection of the human operator of the machine by the reducing the amount of biocide used and reducing of used sources by their longer utilizing (economic, environmental and safety aspects). On the other hand, after the useful life of process fluids on the machine will be monitored the effect of high concentration of O3 (with the combination of other advanced oxidative processes mostly sonolysis and photocatalytical oxidative processes) to accelerating biodegradation of MWFs (economic and environmental aspects). The decrease of organic substances content as well as the primary elimination of biocides will help to biological degradation of this type of waste. Both aims reflect to the world trend of

sustainability, decreasing substances toxicity and increasing of biological treatment of wastes.

Project Title	**The readiness of industrial enterprises to implement the requirements of standards for quality management systems ISO 9001:2015 and environmental management systems ISO 14001:2014**
Coordinator	doc. RNDr. Miroslav Rusko, PhD.
Start Date	01/01/2015
End Date	31/12/2017
Program	VEGA
Annotation	The project is focused on the research and analysis of current approaches to quality management system and environment with respect to readiness to implement the changes induced by formation of SL Annexes to Regulation ISO / EIC "Consolidated Supplement - Procedures specific to ISO", and in particular the requirements into a single structure standards for management systems. Based on the analysis methodology will be created for successful transformation of new approaches to quality management and environmental management as defined in forthcomming revisions of the standards. Besides, the methodology for effective implementation of defined standards requirements will be developed.

Project Title	**Fire safe insulation systems based on natural materials**
Coordinator	doc. Ing. Jozef Martinka, PhD.
Start Date	01/01/2016
End Date	31/12/2018
Program	VEGA
Annotation	The size of a fire is directly proportional to the time elapsed from ignition and conditions of fire development. One of the conditions, increasing fire development, is the presence of combustibles which are prone to ignition and support flame spread and heat release. These include also natural materials which are currently being used increasingly as environmental-friendly thermal insulation in timber frame buildings, but also in traditional construction. The behaviour of these materials in fire is not well defined since they are novel without a history of use. Further aspect of these materials is the fact that they are usually used in combination with other materials, which affects the overall development of fire and may cause difficulties in fire-fighting operations. One of the possible solutions is to rate the fire resistance of the whole panel as required by the standards.

Project	**Title Creation of high schoolbooks for study programmes Fire protection and safety and Integrated safety**
Coordinator	prof. Ing. Karol Balog, PhD.
Start Date	01/01/2016
End Date	31/12/2018

Program KEGA

Annotation The common creation of multimedia university schoolbook by teachers from the universities providing education in related study branches rescue services and labour safety will provide the education enhancement of high-school educated experts. The integration of basic knowledge improves the graduates implementation in praxis and at the same time maintains the diversified profiles of graduates, their specific knowledge and abilities. The university schoolbook multimedia content and the publication of elaborated lectures of the selected subjects and videopresentations of laboratory exercises on the internet pages of the both universities will allow students to manage effectively the study with their individual possibilities in accordance with the principles of the credit system. The university schoolbook will be consist of the key themes of study programmes core subjects. Its selected themes parts will be questions and problems of final exams at the both universities. The project outputs multimedia processing will be suitable mainly as a study materials for the combined and distance study method in the external study programmes and also as an innovative study material for the experts from praxis and non-academic sphere. The selected lectures presentations published in English language will be helpful for students from abroad.

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: Progressive methods of material fire-technical characteristics determination in fire engineering

Coordinator prof. Ing. Karol Balog, PhD.

Start date 24/10/2013

End date 30/09/2017

Programme APVV

Annotation The contribution to research in the area of fire engineering in accordance with world trends by utilisation of the progressive methods for determination of important fire-technical characteristics for calculation and modelling of compartment fires. The characterisation and verification of the laboratory testing methods with modern equipment utilisation for obtaining of the unique material characteristics and their alterations due heat and fire. The behaviour prediction of solid and liquid materials in the process of initiation and propagation of combustion on the ground of the determined characteristics. The application of new methods for determination of critical boundary

conditions of testing of representative materials in the progressive material structures for the improving of outputs from used fire scenarios.

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	**Knowledge discovery for hierarchical control of technological and production processes**
Coordinator	prof. Ing. Pavol Tanuška, PhD.
Start Date	01/01/2015

End Date 31/12/2017
Program VEGA
Annotation The project is aimed at the area of knowledge discovery on databases and the application of such knowledge in hierarchical process control. It will include conceptual design of a knowledge discovery process in hierarchical control systems. The formulation of the proposal design will constitute comprehensive approach to solving problems related to processing of extreme amount of data for the purposes of complex system control. Selected methods of data mining, e.g., based on statistical and inductive learning techniques and chosen on the basis of defined criteria, will be compared in terms of several measurable criteria.

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 **Modernization of the Automatic Control Hardware course by applying the concept Industry 4.0**
Coordinator Ing. Bohuslava Juhásová, PhD.
Start Date 01/01/2016
End Date 31/12/2018
Program KEGA
Annotation The project is focused on the implementation and the use of the Industry 4.0 concept to modernize the syllabus of the course Automatic Control Hardware. A versatile, robust system will be developed Aplikácia konceptu Industry 4.0 v rámci modernizácie predmetu Technické prostriedky automatizovaného riadenia. 3/17 Identifikátor: 20150426231004610 within the project using the latest trends in automation and information technology. The use of the technological concept of the Cyber-Physical System will enable to improve not only the teaching of the subject Automatic Control Hardware, but also other subjects. The developed system could be used in teaching other subjects thanks to the database, which could be possibly complemented by a variety of relevant learning materials. The system will serve to students as well as teachers during the course itself, but also for home self-study. The system will be designed to

support the teacher during the course as much as possible and to teach the students independence and analytical thinking. Another objective of the project is to introduce and teach the students and teachers to use the modern technologies by integrating them into the educational process.

PROJECTS OF THE ADVANCED TECHNOLOGIES RESEARCH INSTITUTE

Project	**Title Searching for physical sources of the fast stochastic oscillations in accreating systems**
Coordinator	Mgr. Andrej Dobrotka, PhD.
Start Date	01/01/2016
End Date	31/12/2018
Program	VEGA
Annotation	The goal of the project is the study of the fast stochastic oscillations generated by turbulent accretion in cosmic objects, where the main driving mechanism is the accretion through a disc. This stochastic flickering usually does not originate only from a single source, hence the light curve is a superposition of more signals. Individual components can be identified by detailed study of the periodogram. For analysis of such complicated periodograms data with high cadence on long time-base are required. Ideal instrument satisfying such demands is the Kepler spacecraft. Its one-minute cadence on time-base over hundreds of days is a unique opportunity for our study. Together with our flickering simulating model based on turbulent accretion process we want to identify individual parts of the complicated periodograms calculated from Kepler telescope data, to localize their source and bring a complex model of accretion in some types of cosmic objects.

Project Title	**High energy heavy ion-beam annealing of ion implantation synthesized silicon carbide**
Coordinator	Ing. Jozef Dobrovodský, CSc.
Start Date	01/01/2016
End Date	31/12/2018
Program	VEGA
Annotation	SiC is a promising material for a wide range of applications from semiconductor industry to e.g. in fuel elements of next generation nuclear power plants' reactors. The most recent method for SiC synthesis is based on carbon implantation into silicon substrate followed by High Energy Heavy-Ion-Beam Annealing (HE HIBA) is currently under development. Advantages of HE HIBA annealing are significantly lower temperature requirements, possibility of localized synthesis and short time of treatment, among other things. Synthesized silicon carbide will be analysed and characterized by Rutherford backscattering spectrometry (RBS), Resonant Nuclear Reaction Analysis (R-NRA), X-ray diffraction (XRD) and transmission electron microscopy (TEM).

Particularly the new experimental facility at MTF STU Trnava equipped with a 500 kV ion implanter and 6 MV tandem accelerator will be utilized. Relation between the main parameters of synthesis processes and of the resulting SiC layers will be studied.

Project Title	**Design of Al-TM alloys for on-board hydrogen production**
Coordinator	RNDr. Martin Šulka, PhD.
Start Date	01/01/2015
End Date	31/12/2018
Program	VEGA
Annotation	The project is aimed on design of Al-TM metal aluminum alloys for on-board hydrogen production by hydrolysis, TM being Co, Ni, Pd, Rh. The goal of the theoretical part is to study the impact of chemical composition on electrochemical stability of aluminum alloys. By periodic DFT we will investigate the influence of chemical composition on electrode potential shift in alloys relative to pure aluminum. We will also examine the segregation of the given element, composition influence on adsorption energies of water and trends in electrochemical stability of alloy surface after the adsorption of water. Within the experimental part we will investigate the correlation between the chemical composition and microstructure of alloys, the influence of preparation conditions and cooling speed on phase composition. Further, we will study the corrosion activity of alloys with emphasis on rapid hydrogen production. Influence of electrolyte type will be evaluated and mechanisms of corrosion will be described.

Project Title	**Physical properties of confined systems**
Coordinator	RNDr. Andrej Antušek, PhD.
Start Date	01/01/2016
End Date	31/12/2018
Program	VEGA
Annotation	An artificial confinement potential is used to model effects of chemical environment of viarious systems. It is widely used for modeling physical phenomena such as in-crystal polarizabilities, electronic structure of quantum dots, high-pressure effects on atoms and molecules and the systems included into nanosized cavities etc.. In our project we will focus on particular problems namely: ab initio calculations of cationic in-crystal polarizabilities, cavity embedded molecules and NMR and hyperfine propeties of semiconductor quantum dots.

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 **C-Au chemical bond in gold ion implanted polyethylene: DFT modeling and experiment**

Coordinator RNDr. Andrej Antušek, PhD.
Start date 01/01/2017
End date 31/03/2018
Programme APVV
Annotation The project is aimed on the theoretical and experimental study of possible C-Au bond creation in gold ion implanted polyethylene. The stability of polyethylene chains with partly Au substituted hydrogen is already confirmed by our preliminary results (theoretical group at ATRI MTF STU). IR spectra of various gold substituted PE chains will be modeled using DFT trying to explain and interpret experimental IR results for gold implanted polyethylene samples prepared in INS Vinca, Serbia. The main chemical and physical properties of the polymers will be predicted by computational chemistry methods.

Project Title **Development of STU research infrastructure**

Coordinator	doc. Ing. Róbert Riedlmajer, PhD.
Start Date	01/01/2017
End Date	31/12/2018
Program	iný domáci
Annotation	The STU´s long-term vision is to strengthen university in international cooperation and other creative activities. That means to strenghten the position of the university in the European research area, to enhance related research infrastructure, to enhance related research infrastructure, to improve the quality of lab equipment and scientific instruments and to improve the spatial conditions also. The project creates a space for immediate scientific cooperation with international partners and partners from industries, enabling more effective transfer of scientific knowledge into practice.