Identification of top research teams of Universities in Slovakia

The Faculty of Natural Sciences presented ten proposals for the assessment of which the Accreditation Commission of the Slovak Republic accepted six top scientific teams. One of these teams is a joint project with the Faculty of Mathematics, Physics and Informatics of Comenius University. The Faculty of Natural Sciences has thus been ranked as the second most successful faculty in Slovakia.

The management of the faculty congratulate all top research teams of our Faculty.

Identified top research teams of the Faculty of Natural Sciences, Comenius University

1. Organic catalysis and other methods of green chemistry (Team name: KATGREEN)

- *Research area*: Organic chemistry
- *Research category according to ISI Web of Knowledge and its classification in the Journal Citation Reports*: a) Chemistry, b) Organic
- *Team researchers*: Doc. RNDr. Martin Putala, PhD., Prof. RNDr. Štefan Toma, DrSc., Doc. Ing. Mária Mečiarová, PhD., Young member of the team: Doc. Mgr. Radovan Šebesta, DrSc.
- *Scope of research*: The team studies and develops methods of green chemistry, especially catalysis of organic reactions. Researchers investigate methodologies of asymmetric catalysis with transition metal complexes, particularly ferrocene and binaphthyl ligands. The team pays attention also to application of small organic molecules, so called organocatalysts in the synthesis of biologically relevant molecules such as drugs oseltamivir, pregabalin and others. In all these topics, the research team is achieving internationally recognized results.

2. Theoretical and computational chemistry (Team name: TEOCHEM)

- *Research area*: Chemistry
- *Research category according to ISI Web of Knowledge and its classification in the Journal Citation Reports*: a) Chemistry, physical; b) Physics, atomic, molecular & chemical; c) Computer science, interdisciplinary applications
- *Team researchers*: Prof. RNDr. Ivan Černušák, DrSc., Prof. RNDr. Vladimír Kellö, DrSc., Prof. RNDr. Jozef Noga, DrSc., Prof. RNDr. Miroslav Urban, DrSc., Doc. Mgr. Pavel Neogrády, Dr., Young members of the team: Mgr. Michal Pitoňák, PhD. a RNDr. Ján Šimunek, PhD.
- *Scope of research*: The TEOCHEM group has been developing quantum chemical ab initio methods since early 1970s. These methods aim to predict the properties of atoms and molecules with controlled accuracy, without using empirical parameters. The most important results were obtained in the realm of electron correlation in atoms, molecules and molecular clusters. The team belongs to first three groups in the world that mastered routine electron correlation calculations up to complete fourth order of diagrammatic perturbation theory, as

well as using the coupled cluster approach including singly-, doubly-, triply- and part of quadruply excited electron configurations. We have significantly contributed to the development of the hierarchy of the CC methods that allow systematic and numerically controlled improvement of atomic/molecular data and increase their computational efficiency. We have implemented this theoretical approach in computer codes Comenius, MUNICH and Molcas. Subsequently, an impressive series of applications has been published by the members of the team: calculations of electric and spectroscopic properties of atoms and molecules, intermolecular interactions and chemical reactivity. These results serve as reference data for less accurate quantum chemical computational approaches. Team also contributed to better understanding of the relativistic effects in atomic/molecular properties, especially when heavy atoms are present. These applications pave the route to understand the extraordinary properties of nano-clusters and their interactions with various ligands, and to model the processes at surfaces or in bio-systems. Modelling the properties and interactions in silico for biomolecules can lead to biomedical applications. Another important topic is thermo-kinetic calculations and modelling in environmental chemistry, in particular the studies of gas-phase chemistry of troposphere and stratosphere. The group cooperates with world top-laboratories in the field of theoretical chemistry (Quantum Theory Project, University of Florida, USA, Lund University, Sweden, University of Lille, France, Institute of organic chemistry and biochemistry AVČR, Czech Republic, Massey University, New Zealand). Team is participating also in the Horizon 2020 research program within Eurofusion project. Integral parts of our work are also research activities of our students who regularly participate in the Student's scientific conference at our university. Traditionally, the students of master and doctoral degree spend some time at our partner institutions abroad or at summer/winter schools of theoretical chemistry. From the academic year 2016/2017 we launch the prestigious fellowship for the best master/PhD students in theoretical chemistry. Many of results/publications represent a breakthrough in the field. As an appreciation of our pioneering work two members of the team Miroslav Urban and Jozef Noga were elected as members of prestigious International Academy of Quantum Molecular Science. Our young colleague, Michal Pitoňák, was awarded as the Young researcher of Slovakia in the year 2014 and also by the Literary Fund prize in 2015 for extraordinary annual citation response. In addition, Miroslav Urban, Pavel Neogrády and Michal Pitoňák were awarded by the Literary Fund prize for the top-citation on single publication in 2015. Our PhD student, Michal Novotný, has been awarded by Fulbright fellowship at Stony Brook University (New York) for academic year 2015/2016. Thanks to very good contacts with our partners worldwide it has become a good tradition that our graduates have the chance to work as post-docs at prestigious universities.

3. Invasion Biology and Ecomorphology of Fishes (Team name: IBEF)

- *Research area*: Life Sciences
- *Research category according to ISI Web of Knowledge and its classification in the Journal Citation Reports*: a) Fisheries, b) Zoology
- *Team researchers*: Prof. RNDr. Vladimír Kováč, CSc., Young members of the team: RNDr. Eva Záhorská, PhD., Doc. PaedDr. RNDr. Stanislav Katina, PhD., RNDr. Andrea Novomeská, PhD.
- *Scope of research*: Most of research activities of the IBEF team are devoted to biological invasions, ontogeny, ecomorphology, ecology and phenotypic plasticity of fishes. Biological invasions represent a hot topic of ecology all over the world, being considered a global environmental problem. The range of negative consequences of bio-invasions encompass

issues at the local, national and international levels, including endemic species extinctions, serious economic losses and threats to human health. Fishes also belong to successful invaders, and the invaded areas represent excellent in-situ labs for investigations on adaptations of organisms to novel environments. The IBEF team has contributed to general understanding of some principles that govern ontogenetic processes, as well as biological invasions, with fishes as model organisms. Concerning ontogenetic processes, the key achievement of the IBEF team represents the Theory of synchrony and heterochrony in ontogeny. This theory highlights the importance of two timing mechanisms essential to ontogeny of multicellular organisms – synchrony (coordinating) and heterochrony (implementing). At least three levels of heterochrony should be distinguished: interspecific, intraspecific and intra-individual. This notion widens the former perception of heterochrony as a phenomenon associated almost exclusively with evolutionary processes to understanding heterochrony as one of the key components that affects the existence of life in a much wider scale than previously believed. Thus, the Theory of synchrony and heterochrony in ontogeny has implications for both developmental and evolutionary biology. Concerning biological invasions, the key achievement of the IBEF team is represented by the Theory of alternative ontogenies and invasive potential that explains why some species may become successful invaders whereas other species will not. The novelty of this theory is in its original approach that combines developmental biology with invasion ecology: it focuses on the organism itself rather than on general ecological perspectives. Furthermore, it hypothesizes that epigenetic mechanisms (i.e. environmentally controlled expression of genes) lie behind the developmental plasticity of the successful invaders, which shows the direction for future research. In 2012, the independent ARRA agency identified the IBEF team as a top team of the Comenius University that falls within the top 1 % in the world in the field of study „Plant and Animal Sciences“ http://www.arra.sk/spickove-vedecke-timy-jednotlivci-na-uk-2012. Besides the team leader, professor Vladimír Kováč, the IBEF team consists almost exclusively from young researchers (below 35): Stanislav Katina, Eva Záhorská, Andrea Novomeská. Within the Department of Ecology, several young researchers and/or PhD students participate at the team research activities: Barbora Števove, Kristína Hôrková, Kristína Švolíková and Katarína Jakubčinová. Former PhD students of the team leader (Jozef Tomeček, Mária Balážová, Mária Čápová-Plachá, Daniel Gruľa) also contributed considerably to the team work. Among numerous international collaborators of the IBEF team, professor Gordon H. Copp (Centre for Environment, Fisheries and Aquaculture Sciences, United Kingdom) keeps the leading position.

4. Integračná animálna biológia (Team name: IAB)

- *Research area*: Life Sciences
- *Research category according to ISI Web of Knowledge and its classification in the Journal Citation Reports*: Biology
- *Team researchers*: Prof. RNDr. Michal Zeman, DrSc., Doc. Mgr. Iveta Herichová, PhD., Doc. RNDr. Lucia Kršková, PhD., Young members of the team: RNDr. Katarína Stebelová, PhD., Mgr. Monika Okuliarová, PhD.
- *Scope of research*: Members of the team belong to one department and are key persons who determine research and teaching at the Department of Animal Physiology and Ethology. They supervise doctoral studies at the Department and more than 50 students from the Department and Institutes of Slovak Academy of Sciences successfully defended their doctoral thesis in this field. Two young members are former PhD. students of prof. Zeman, they publish their studies in well recognized international Journals and all together form a

modern chronobiological research, that is highly regarded in Slovakia and abroad. In addition to chronobiological aspects the team recently focuses on the integrative biology and especially of mechanisms underlying animal development and behaviour. Investigation of mutual interactions in physiological control mechanisms is the key feature of the team. The research is supported by projects from national grant agencies (APVV, VEGA) and international programs (COST, bilateral programs). Modern research technologies, young and dynamic team at the department together with a broad scientific cooperation (Medical University of Vienna, Austria, INRA Tours, France, University of Zurich, Switzerland) represent positive pre-conditions for further progress of the team.

5. Research team of the Western Carpathian geodynamics (Team name: GEODYNAMICS)

- *Research area*: Earth and Space Sciences
- *Research category according to ISI Web of Knowledge and its classification in the Journal Citation Reports*: a) Geology, b) Geosciences
- *Team researchers*: Prof. RNDr. Michal Kováč DrSc., Prof. RNDr. Dušan Plašienka, DrSc., Prof. RNDr. Miroslav Bielik, DrSc., Prof. RNDr. Jozef Minár, CSc., Young member of the team: Mgr. Monika Šulc Michalková, PhD. at PhD.
- *Scope of research*: Comprehensive modern research of Western Carpathian geodynamic evolution is the main topic of this team; forming during ESF projects EEDEN (Evolution and Ekosystems dynamics of Euroasian Neogene), EUROCORES TOPO-EUROPE and CELEBRATION 2000. Reconstructions and models are supported by the geophysical research of the Earth lithosphere on one side and by investigation of the surface manifestation of geodynamic processes in landforms and recent geomorphic processes on the other side. Unique interdisciplinary geological, geophysical and geomorphological approach leads to innovative outcomes. Original definition of ALCAPA and Tizsa Dacia microplates (the first application of new paradigmatic microplate theory in the region) and subsequent paleogeographical reconstructions in the European scale formed a basis for pioneer interpretations. Models of basic geophysical discontinuities and anomalous bodies, new tectonic sudivision of the Western Carpathian orogen in context of the Alpine systems, and its new morphostructural subdivision are the other achievements. At 13th Congress of the Regional Committee on Mediterranean Neogene Stratigraphy, leader of the team Michal Kováč was awarded in recognition of his fundamental contribution to the understanding of the Paratethys geodynamics. The young team member Monika Šulc Michalková was selected as the only representative of French and Slovak geomorphology school for preparation of "whitepaper" – Dynamic interactions of life and its landscape: feedbacks at the interface of geomorphology and ecology (programme MYRES, New Orleans, USA).

6. Mineralogical-Petrologic team in Geological Sciences (Team name: MPT)

- *Research area*: Geology, Mineralogy, Petrology
- *Research category according to ISI Web of Knowledge and its classification in the Journal Citation Reports*: a) Geology, b) Mineralogy
- *Team researchers*: Prof. RNDr. Marián Putiš, DrSc., Prof. RNDr. Pavel Uher, CSc., Doc. Mgr. Martin Ondrejka, PhD., Young member of the team: Doc. RNDr. Peter Bačík, PhD.
- *Scope of research*: Members of the team belong to establishing members of the Centre of excellence for research and education of solid phase focused on nanomaterials,

environmental mineralogy and material science (SOLIPHA). They use microscopic, electron-optic, X-ray diffraction and spectroscopic methods for the research of minerals and rocks, and for reconstruction and isotopic dating of magmatic and metamorphic processes in crustal and mantle lithosphere. They performed new practical experiments on enhancement of optical properties of some gem minerals with detailed study of crystal-chemical properties with the influence on colour. New development studies are aimed to biomineralogy and analysis of particulate matter in atmospheric dust. Members of the team systematically present project results at International Geological Congresses and Conferences. They are often invited for lectures by well-known universities and geological/mineralogical societies. The team members participate in international scientific working groups. They supervised many diploma and doctoral students, the best of which are successful scientists at universities abroad or they are contracted with prestigious private geological enterprises. Key achievements: The team has contributed to the integrated study of crustal-scale shear zones in the Western Carpathians and Eastern Alps by using the petro-tectonic methods. They revealed mechanical models of rock exhumation in deep-seated mobile zones of the Earth crust based on study of mineral preferred-orientation patterns of mylonitic rocks from the shear zones. They discovered new interaction systems between fluids and rocks in subduction-related accretionary wedges - e.g., in published case studies about the Neotethyan Meliata tectonic Unit. Many applications of isotopic geochronological methods, including SIMS-SHRIMP and LA-ICP-MS, represent a pioneering contribution to geochronology of the Western Carpathians and Eastern Alps. The latter methodology results represent a comprehensive database used not only in the Alpine-Carpathian mountain range but also for the world-wide paleotectonic and geodynamic models reconstructions. As an example, the definition of the oldest Gondwana paleocontinent remnants discovered in our territories according to dated zircon age of 3.4 billion years obtained from a granitic orthogneiss in the Vepor Mountains, can be used. Thermodynamic modelling of magmatic and metamorphic processes contributed to original knowledge on crust-mantle lithosphere interaction. Mineralogy studies are aimed to revealing potential sources of so-called critical metals, especially minerals of the rare litophile elements (REE, Nb, Ta, Zr, Hf and others). The study has been focused on crystal chemistry, structure, internal zoning, dating and alteration of monazite, xenotime, apatite, allanite, zircon, garnets, tourmalines, and Nb-Ta oxide minerals as key accessory phases, indicators of the host-rock evolution. Original discoveries of our team comprise first time defined metamorphic-metasomatic perovskite genesis, or definition oxy-schorl as a new mineral of tourmaline group. Research in crystal chemistry brought many interesting discoveries, new substitution relationships have been discovered in REE phosphate-arsenate minerals, minerals of tourmaline and epidote groups. Similarly, mechanisms incorporating some potentially risk elements like S, As, Sr, U, and Th in monazite structure were explained.